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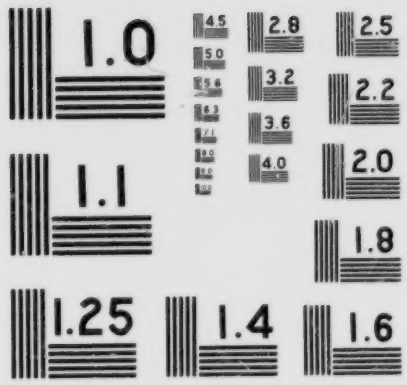

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MATHEMATICAL URBAN AIR POLLUTION MODELS

by

Harry Moses

ARGONNE NATIONAL LABORATORY

ENVIRONMENTAL SCIENCES

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April 1969

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ABSTRACT

MATHEMATICAL URBAN AIR POLLUTION MODELS

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This paper provides a review of the use of mathematical models for urban air pollution problems. Discussed are the major contributions in this field beginning with the early work of Frenkiel to those of modern day operational models. Too allow an assessment of work in this area, five tables are presented including the locations of the studies, types of tracers, sizes of the monitoring and meteorological networks, amounts of data collected, and the mathematical equations used.

The urban air pollution model is considered as having four components. These are:

1. the source inventory, including point as well as area sources,
2. the network of meteorological stations,
3. the network of pollutant monitoring stations, and
4. the mathematical algorithm which describes the processes which transform the concentrations at the source to those observed at the receptor.

Also, a substantial amount of attention is devoted to verification procedures.

Two general categories of mathematical models are discussed. The first is the source-oriented model characterized by the work of Turner. In this model, the concentration at a particular point is determined by the superposition of the contributions from each of the sources upwind. The second is the receptor-oriented model of which there are three types: the first is that described by Clarke, in which

the pollutant concentrations at a particular monitoring station are analyzed in a manner similar to that of the source-oriented model. Second, there is the regression model, in which regression equations are developed relating observed concentrations at a receptor with meteorological variables; and third, the Tabulation Prediction Scheme in which combinations of meteorological variables are arranged in an ordered sequence. For each combination, the probability distribution of pollutant concentration is given along with other statistical parameters such as the interquartile range, the mean, and the standard deviation of the distributions. With the tabulation prediction scheme, one may look up the meteorological conditions just as one looks up a name in a telephone book or a word in a dictionary and read off the probability distribution of concentrations.

A summary of verification techniques is given with examples of how other workers in the field have verified their models. These include scatter diagrams, correlation coefficients, and isopleth comparisons. The weaknesses and strengths of validation techniques are discussed.

MATHEMATICAL URBAN AIR POLLUTION MODELS

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I. INTRODUCTION

The undesirable effects of air pollution emphasizes the need for understanding the role played by the atmosphere in affecting the levels of pollutant concentration. With a constant rate of emission into the atmosphere, concentrations on the ground may be 1000 times greater under the poorest conditions than under the most favorable ones. For this reason, the role of meteorology in air pollution has been receiving increasing attention.

A mathematical air pollution model may serve to gain insight into the relation between meteorological elements and air pollution. It may be likened to a transfer function where the input consists of both the combination of weather conditions and the total emission from sources of pollution, and the output is the level of pollutant concentration observed in time and space. The mathematical model takes into consideration not only the nature of the sources, (whether they are distributed or point sources) and the levels of concentration at the receptors, but also the atmospheric processes which take place in transforming the concentrations at the sources of emission into those observed at the receptor or monitoring station. Among such

processes are photochemical action, adsorption either on aerosols or ground objects, and of course, eddy diffusion.

There are a number of areas in which a valid and practical model may be of considerable value. For example, the operators of an industrial plant which will emit sulfur dioxide want to locate it in a particular community. Knowing the emission rate as a function of time, the distribution of wind speed, wind direction, and atmospheric stability, the location of SO_2-sensitive industrial plants, and the spatial distribution of residential areas, it is possible to calculate the effect the new plant will have on the community. As air quality standards are developed, one may intelligently place limits on the amount of emission allowed to any industrial group.

In large cities, such as Chicago, Los Angeles, or New York during strong anticyclonic conditions with light winds and low dispersion rates, pollution levels may rise to a point where health becomes affected; eyes smart, hospital admissions for respiratory ailments increase, and in some cases even deaths result. To minimize the effects of air pollution episodes, advisories or warnings are issued by government officials. Tools for determining, even only a few hours in advance that unusually severe air pollution conditions will arise are invaluable. The availability of a workable urban air pollution model plus a forecast of the wind and stability conditions could provide the necessary information.

In long range planning for a growing community, it may be desirable to zone some areas for industrial activity and others for residential use in order to minimize the effects of air pollution. Not only the average sized community, but also the large megalopolis

could profitably utilize the ability to compute concentrations resulting from given emissions using a model and suitable weather data. In addition, the establishment of an air pollution climatology for a city or state which can be used in the application of the model would represent a step forward in assuring clean air.

For all these reasons, a number of groups have been devoting their attention to the development of mathematical models for determining how the atmosphere disperses materials.

II. HISTORY OF MATHEMATICAL MODEL DEVELOPMENT

The pioneer in this work is Dr. Francois N. Frenkiel [1] who developed a mathematical model for the city of Los Angeles. After Frenkiel's early work, the problem was taken up by the Meteorology Group of the Public Health Service at the Robert A. Taft Sanitary Engineering Center in Cincinnati, Ohio under the direction of Mr. Robert A. McCormick. The Meteorology Group of the Robert A. Taft Sanitary Engineering Center is now part of the National Air Pollution Control Administration of the Department of Health, Education and Welfare.

Turner [2] laid the foundation for daily operational models in his development of the Nashville model. Later this group performed an extensive air pollution study of the St. Louis area. Turner extended and improved his Nashville model for application to this investigation. Pooler [3] has carried out nine series of measurements over St. Louis to study the nature of urban atmospheric diffusion. Clarke [4] another member of the team used measurements over Cincinnati to produce a rather simple model for this area. Still another group, Miller and Holzworth [5], developed a new model

which depends heavily on the mixing layer concept. Schiermeier [6] carried out further tests and refinements on the Clarke model for St. Louis, and Kussman [7, 8] tested and refined both the Clarke model and Miller and Holzworth model for New York City.

Simultaneously, work on air pollution models progressed at a number of universities: 1. a group at the University of Florida [9] developed a model for the city of Jacksonville, Florida, 2. Pennsylvania State University [10] developed a model for Johnstown, Pennsylvania, 3. New York University [11] developed a very sophisticated model for New York City. New York City has over 100 wind measuring stations. This group obtained substantial amounts of data on the variation of SO_2 as well as temperature with height by means of a helicopter.

An advance in this problem resulted from the work at the Travelers Research Center [12], performed by Professor Franklin I. Badgley, on leave from the University of Washington, Dr. Glenn Hilst and other staff members. They developed a model for the state of Connecticut. Concentration measurements are currently being obtained to test this model. The theory was developed to a rather high degree. Hilst and Bowne [13] of the Travelers Research Center carried out another study to develop a diffusion model over Fort Wayne, Indiana based on an elevated line source emitted from an aircraft.

An urban model study outside of the United States has been that of Fortak for the city of Bremen [14]. He also was concerned with the SO_2 problem.

A listing of the investigations dealing with urban air pollution models on which this paper in based is given in Table I. The tabu-

lation gives the authors, locations, and pollutants used. To allow an assessment of the magnitude of each program, Tables II, III and IV are presented. Table II shows the duration of the study, the date of publication, and information on the amount of data obtained. Table III provides information on the size of the meteorological and pollution monitoring stations, while Table IV presents characteristic features of the model: sample duration, nature of the grid networks, and effective plume heights.

One of the most extensive efforts in the development of an urban air pollution model for SO_2 is that of the Argonne National Laboratory made in collaboration with the City of Chicago and sponsored both by the Department of Health, Education and Welfare and the Atomic Energy Commission [15, 16, 17]. Available for this study are over three years of data consisting of 15-minute readings from eight stations providing information on SO_2 concentrations, wind speed, and wind direction. Details and the results on its program are discussed elsewhere [15, 16, 17].

The above models were designed to provide daily or hourly values of concentrations at selected points over a city. Models to provide monthly or seasonal values of pollution concentrations have also been devised. Pooler [18] and Meade and Pasquill [19] describe such models. Pooler calculated monthly averages of SO_2 concentration for Nashville using a network of 123 lead peroxide candles. Meade and Pasquill had available the data from a 14-station network also equipped with lead peroxide candles. Their model determined seasonal averages of SO_2 concentrations in the vicinity of the Staythorpe electric power station in England.

III. COMPONENTS OF AN URBAN AIR POLLUTION MODEL

A mathematical urban air pollution model comprises four essential components. The first is the source inventory. One must know what materials, how much, from what location, and at what rate they are being injected into the atmosphere or what is being brought into a community across the boundaries. The second involves the measurement of contaminant concentration at representative parts of the city, sampled properly in time as well as space. The third is the meteorological network, and the fourth is the meteorological algorithm or mathematical formula which describes how the source input is transformed into observed values of concentration at the receptors. See Figure 1. The difference between what is actually going on in the atmosphere and what we think goes on, based on our measured sources and our imperfect mathematical formulations as well as our imperfect sampling of air pollution levels, causes discrepancies between the observed and calculated values.

Also of importance is the verification procedure. The remainder of this paper is devoted to these four components and the verification procedures.

Accounts may be found in the literature of a number of investigations which do not have the four components of the mathematical urban air pollution model mentioned above, namely, the source inventory, the mathematical algorithm, the meteorological network, and the monitoring network. Some of these have one or more of the components missing. An example of this kind is the theoretical investigation such as that of Lucas [20] who developed a mathematical technique for determining the pollution levels of sulfur dioxide produced by the thousands of domestic fires in a large city. No measurements are presented to support this study. Another is that of Slade [21] who discusses a megalopolis model. Smith [22] also presented a

theoretical model which is essentially an urban box model. Another is that of Bouman and Schmidt [23], on the growth of pollutant concentrations in the cities during stable conditions. Three case studies, each based on data from a different city, are presented to support these theoretical results. Studies relevant to the urban air pollution problem are the pollution surveys such as the London survey [24], the Japanese survey [25], and that of the Capitol region in Connecticut [26]. In these studies, analyses are made of pollution measurements; and in some cases meteorological as well as source inventory information are available; but in most cases, the mathematical algorithm for predicting pollution is absent. Another study of this type is one on suspended particulate and iron concentrations in Windsor, Canada by Munn, Thomas, and Cole [27]. Early work on forecasting urban pollution is described in two papers: one by Scott [28] for Cleveland, Ohio and the other by Kauper, Hartman, and Hopper [29] for Los Angeles, California. A comparison of urban models has been made by Wanta [30] in his refreshing article which discussed the relation between meteorology and air pollution.

IV. THE SOURCE INVENTORY

In the development of an urban air pollution model, two types of sources are considered: (1) individual point sources, and (2) distributed sources. The individual point sources are often the large coalburning power generating station stacks or the stacks of large buildings such as the Chicago Merchandise Mart. Any chimney stack may serve as a point source, but some investigators have placed lower limits on the emission rate of a stack to be considered a point souce in the model. Fortak [14], for example, considers

a source as an individual point source if it emits 1 kgm of SO_2 per hour, while Koogler et al. use a 10-kgm-per-hour criterion [9]. In addition, when ground concentrations are calculated from the emission of an elevated point source, the effective stack height must be determined, i.e., the actual stack height plus the additional height due to plume rise.

Information concerning emission rates, emission schedules, or per cent of sulfur is customarily obtained by means of a source inventory questionnaire. It is usual to find the answering rate of such questionnaires quite low. A municipality with licensing power, however, has the advantage of being able to force disclosure of information provided by a source inventory questionnaire since the license may be withheld until the desired information is furnished. Merely the awareness of this capability is sufficient to result in gratifying cooperation. The City of Chicago has received a very high percentage of returns from those to whom a source inventory questionnaire was submitted.

Information on distributed sources may be obtained in part from questionnaires, and, in part, from an estimate of the population density. Population density data may be derived from census figures or from an area survey employing aerial photography.

In addition to knowing where the sources are, one must have information on the rate of emission as a function of time. Information on the emission for each hour would be ideal, but nearly always one must settle for much cruder data. Usually one has at his disposal for use in the calculations only annual or monthly emission rates. Corrections for diurnal patterns may be applied, i.e., more coal is

burned in the morning when people arise than during the latter part of the evening when most retire. Roberts [15] has referred to the relationship describing fuel consumption (for domestic or commercial heating) as a function of time, e.g., the hourly variation of coal use, as the "janitor function." Consideration of changes in hourly emission patterns with season is, of course, also essential.

In addition to the classification involving point sources and distributed sources, the source inventory information is often stratified according to broad general categories to serve as a basis for estimating source strengths. The nature of the pollutants - e.g., whether it be sulfur dioxide or lead - influences the grouping. Frenkiel [1] has described his sources as those due to: (1) automobiles, (2) oil and gas heating, (3) incinerators, and (4) industry; Turner [2] has used the categories: (1) residential, (2) commercial, and (3) industrial; the Connecticut model [12] considers these classes: (1) automobiles, (2) home heating, (3) public services, (4) industrial, and (5) electric power generation. (Actually, the Connecticut model had a number of subgroups within these categories.) In general, each investigator used a classification tailored to his needs and one which faciliated estimating the magnitude of the distributed sources.

Source inventory information is difficult to acquire to the necessary level of accuracy; nevertheless, it forms an important component of the urban air pollution model.

V. THE MATHEMATICAL EQUATIONS

Mathematical equations of urban air pollution models describe the processes by which pollutants injected into the atmosphere are

diluted. A number of mathematical formulations may be used to describe the atmospheric diffusion process, but the one which enjoys the widest use is a form of the Gaussian equation, also referred to as the modified Sutton equation. In its simplest form for a continuous ground level point source, it may be expressed as

$$\frac{\chi}{Q} = \frac{1}{\pi u \sigma_y \sigma_z} \exp\left(- \frac{y^2}{2\sigma_y^2} - \frac{z^2}{2\sigma_z^2} \right) \quad (1)$$

χ = Concentration in grams/meter^3

Q = Grams per second

u = Wind speed at the emission point in meters/second

σ_y = The perpendicular distance in meters from the centerline of the plume in the horizontal direction to the point where the concentration falls to 0.61 times the centerline value.

σ_z = The perpendicular distance in meters from the centerline of the plume in the vertical direction to the point where the concentration falls to 0.61 times the centerline value.

π = 3.1416

x, y, z = Spatial coordinates - downwind, crosswind, and vertical distances respectively with the origin at the point source.

Any consistent system of units may be used.

From an examination of the variables it is readily seen that several kinds of meteorological measurements are necessary. The wind speed, u, appears explicitly in the equation; the wind direction is necessary for determining the direction of pollutant transport from source to receptor.

Further, the values of σ_y and σ_z depend upon atmospheric stability which in turn depends upon the variation of temperature with

height, another meteorological parameter. At the present time, data on atmospheric stability over large urban areas are uncommon. Pasquill has developed Table VI for use with Figures 2 and 3, as a substitute for stability measurements to determine values of σ_y and σ_z. Turner [2] has proposed a modification of the Pasquill diagrams for the same purpose. Panofsky and Prasad [10] have used the range of the direction swings of a wind vane as a substitute of values of σ_y and σ_z.

The temperature variation with height may be obtained by means of thermal elements mounted on radio or television towers. Tethered or free balloons carrying suitable sensors may also be used. Helicopter soundings of temperature have been used for this purpose in New York City, Cincinnati, Ohio and elsewhere. There is little doubt that as additional effort is devoted to the development of urban air pollution models, adequate stability measurements will become available. In a complete study, measurements of precipitation, solar radiation, and net radiation flux may be used to advantage. Another meteorological variable of importance is the hourly temperature for hour-to-hour predictions or the average daily temperature for 24-hour calculations. The source strength, Q, when applied to an area source consisting of residential units burning coal for space heating, is a direct function of the number of degree hours or degree days. The number of degree days is defined as the difference between the average temperature for the day and 65°. If the average temperature exceeds 65°, the degree day value is considered zero. An analogous definition applies for the degree hour. Turner [31] points out that in St. Louis the degree day or degree hour values explain nearly

all the variance of the output of gas as well as of that of steam produced by the public utilities.

VI. THE USE OF GRIDS

In the development of a mathematical urban air pollution model, two different grids may be used: one based on existing pollution sources and the other on the location of the instruments which from the monitoring network.

A. The Pollution Source Grid

In this country, grid squares, one mile on a side are frequently used, such as was done by Davidson, Koogler, and Turner. Fortak of West Germany used squares, 100 x 100 meters. The Connecticut model is based on a 5000-foot grid, and Clarke's Cincinnati model on sectors of a circle. Sources of pollution may be either point sources such as the stacks of a public utility, or distributed sources such as the sources representing the emission of many small homes in a residential area. The map of Fig. 4 shows the pollution source grid for the City of Chicago.

B. The Monitoring Grid

In testing the model, one resorts to measurements obtained by instruments at monitoring stations. Such monitoring stations may also be located on a grid. Further, this grid may be used in the computation of concentrations by means of the mathematical equation, e.g., concentrations are calculated for the midpoints of the grid squares. The emission grid and monitoring grid may be identical or they may be different. For example, Turner used a source grid of 17 x 16 miles, but a measurement grid of 9 x 11 miles. In the Connecticut model, the source grid covers the entire state, and cal-

culations based on the model also cover the entire state. Fortak used 480 x 800 meter rectangles.

VII. TYPES OF URBAN AIR POLLUTION MODELS

A. The Source-Oriented Model

In applying the mathematical algorithm, one may proceed by determining the source strength for a given point source and then calculating the isopleths of concentration downwind arising from this source. The calculation is repeated for each area source and point source. Contributions made by each of the sources at a selected point downwind such as the midpoint of square 15 in Fig. 5, are then summed to determine the calculated value of the concentration. Isopleths of concentration may then be drawn to provide a computed distribution of the pollutants.

In the source-oriented model, detailed information is needed both on the strength and on the time variations of the source emissions. The Turner model [2] is a good example of a source-oriented model.

It must be emphasized that each urban area must be "calibrated," to account for the peculiar characteristics of the terrain, buildings, forestation, and the like. Further, local phenomena such as lake-breezes and mountain-valley effects may markedly influence the resulting concentrations. Specifically, one would have to determine such relations as the variation of σ_y and σ_z with distance or the magnitude of the effective stack heights. A network of pollution monitoring stations is necessary for this purpose. The use of an algorithm without such a calibration is likely to lead to disappointing results.

B. The Receptor-Oriented Model

Several types of receptor-oriented models have been developed. Among these are the Clarke model, the regression model, and the Argonne tabulation prediction scheme.

1. The Clarke Model

In the Clarke model [4], one of the most well-known, the receptor or monitoring station is located at the center of four concentric circles having radii of 1, 4, 10, and 20 kilometers respectively. These circles are divided into 16 equal sectors of 22 1/2°. See Fig. 6. A source inventory is obtained for each of the 64 (16 x 4) annular sectors. Also for the 1-km radius circle and for each of the annular rings, a chart is prepared relating $\frac{\chi}{Q}$ (the concentration per unit source strength) and wind speed for various stability classes and for various mixing heights. The algorithm such as given in Table V for the Clarke model may be used. An example of such a chart is shown in Fig. 7. In refining his model [32], Clarke considers, separately, the contributions to the concentration levels made by transportation, industry and commerce, space heating and strong point-sources such as utility stacks. The following equations are then used to calculate the pollutant concentration.

$$\chi_T = \sum_{i=1}^{4} (\chi/Q)_{Ti} \; Q_{Ti}$$

$$\chi_I = \sum_{i=1}^{4} (\chi/Q)_{Ii} \; Q_{Ii}$$

$$\chi_S = \sum_{i=1}^{4} (\chi/Q)_{Si} \; Q_{Si}$$

$$\chi_{Total} = a\chi_T + b\chi_I + c\chi_S + \sum_{i=1}^{n} k_i\chi_p$$

χ = Concentration in grams/cubic meter

Q = Source strength in grams/sec

T = Subscript to denote transportation sources

I = Subscript to denote industrial and commercial sources

S = Subscript to denote space heating sources

p = Subscript to denote point sources

i = Refers to the annular sectors

The above equations with some modification are taken from Clarke's report [32]. Values of the constants a, b, c are determined from information concerning the diurnal variation of the transportation, industrial and commerical, and space heating sources. The coefficient, k_i, represents a calibration factor applied to the point sources.

2. The Linear Regression-Type Model

A second example of the receptor-oriented model is one developed by Roberts and Croke [17] using regression techniques. Here,

$$\chi = C_0 + C_1Q_1 + C_2Q_2 + \sum_{i=1}^{n} k_iQ_i$$

In applying this equation, it is necessary first to stratify the data by wind direction, by wind speed, and by time of day. C_0 represents the background level of the pollutant; Q_1 represents one type of source such as the commercial and industrial emissions and Q_2 may represent emissions due to home space heating. The k_iQ_i terms represent contributions due to large individual point sources. It is assumed that there are n point sources. The coefficients C_1 and C_2 and k_i represent the $\frac{1}{\sigma_y\sigma_z}$ term as well as the contribution

of the exponential factor of the Gaussian type diffusion equation. See Equation 1.

Multiple discriminant analysis techniques [17] for individual monitoring stations may be used to determine the probability that pollutant concentrations fall within a given range or that they exceed a given critical value such as 0.3 ppm. Meteorological variables, such as temperature, wind speed, and stability are used as the independent variables in the discriminant function.

3. The Tabulation Prediction Scheme

This method, developed at the Argonne National Laboratory, consists of developing an ordered set of combinations of relevant meteorological variables and presenting the percentile distribution of SO_2 concentrations for each element in the set. An example of the tabulation is shown in Table VII. In this table, the independent variables are wind direction, hour of day, wind speed, temperature, and stability. The 10, 50, 75, 90, 95, 98 and 99 percentile values are presented as well as the minimum and the maximum values. Also presented are the interquartile range and the 75-95 percentile ranges to provide a measure of dispersion and of skewness respectively.

Since the meteorological variables are ordered, it is possible to look up any combination of meteorological variables just as one would look up a name in a telephone book or a word in a dictionary. This method, of course, can be applied only as long as the source distribution and terrain have not changed appreciably. For continued use of this method, one must be cognizant of changes in the sources as well as changes in the terrain due to new construction.

In preparing the tabulation, the data are first stratified by

season and also by the presence or absence of precipitation. Further, appropriate group intervals must be selected for the meteorological variables to assure that within each grouping the pollution values are not sensitive to changes in that variable. For example, becuase of the spatial distribution of the sources, one finds that the pollution concentration at a station varies markedly with changes in wind direction. If one plots percentile isopleths for concentration vs. wind direction, see Fig. 9, one may choose sectors in which the SO_2 concentrations are relatively insensitive to direction change. A similar chart to determine time bands during which SO_2 concentrations are insensitive to the hour of the day is shown in Fig. 8. With the exception of wind direction and hour of day, the meteorological variables of Table VII vary monotonically with SO_2 concentration.

The tabulation prediction method has advantages over other receptor-oriented techniques in that (1) it is easier to use, (2) it provides predictions of pollution concentrations more rapidly, (3) it provides the entire percentile distribution of pollutant concentration to allow a forecaster to "fine tune" his prediction based on synoptic conditions, and (4) it takes into account nonlinearities in the relationships of the meteorological variables and SO_2 concentrations. In a sense, one may consider the tabulation as representing a nonlinear regression hypersurface passing through the data which represent points plotted in n-dimensional space. The analytic form of the hypersurface need not be determined in the use of this method.

The disadvantages of this method are that (1) it is necessary to have the use of a large digital computer in constructing the

tables, (2) at least two years of meteorological data are necessary, (3) changes in the emission sources degrade the method, and (4) the model could not predict the effect of adding, removing or modifying important pollution sources; however, it can be designed to do so.

Where a network of stations is available such as exists in New York City, Los Angeles, or Chicago, then the receptor-oriented technique may be applied to each of the stations to obtain isopleths of concentration similar to that obtained in the source-oriented model.

It would be ideal to have a source-oriented model which could be applied to any city, given the source inventory. Unfortunately, the nature of the terrain, general inaccuracies in source strength information and the influences of factors such as synoptic effec or the peculiar geometries of the buildings produce substantial errors. Similarly, a receptor-oriented model, such as the Clarke model or one based on regression techniques must be tailored to the location. Every urban area must therefore be "calibrated" whether one desires to apply a source-oriented model, or a tabulation prediction scheme. The tabulation prediction scheme, however, does not require detailed information on the distribution and the strength of emission sources.

Perhaps, the optimum system would be one which would make use of the advantages of both the source-oriented model with its prediction capability concerning the effects of changes in the sources and the tabulation prediction scheme which could provide the probability distributions of pollutant concentrations. It appears possible to develop a hybrid system by developing means for appropriately

modifying the percentile entries when sources are modified, added or removed. The techniques for constructing such a system would, of course, have general applicability.

VIII. ADAPTION OF BASIC EQUATION TO URBAN AIR POLLUTION MODELS

The basic equation, Equation 1, is the continuous point source equation with the source located at the ground. It is obvious that the sources of an urban complex are for the most part located above the ground. The basic equation must, therefore, be modified to represent the actual conditions. Table V shows the mathematical algorithms used by various authors and includes appropriate modifications of Equation 1.

A. Removal of Pollutants

When one considers a gaseous pollutant such as SO_2, he must account for its continuous removal from the atmosphere by a number of processes. For example, in the presence of manganese dioxide, acting as a catalyst, SO_2 oxidizes to SO_3 which in turn becomes H_2SO_4. Sulfuric acid may react with ammonia to form $(NH_4)_2SO_4$. Other sulfates may be formed which absorb water, increase in size, and fall to the ground. If precipitation is occurring, then rainout or washout may remove the SO_2 during the transport between the source and the receptor.

Further, SO_2 may become absorbed by vegetation or other materials at the ground surface.

If one makes the assumption that the removal rate is directly proportional to the amount of pollutant present then

$$\frac{dX}{dt} = -\lambda X$$

or integrating between the indicated limits, one has

$$\int_{\chi_o}^{\chi} \frac{d\chi}{\chi} = -\int_o^t \lambda dt$$

or

$$\chi = \chi_o e^{-\lambda t} = \chi_o \exp - \frac{0.693t}{T_{1/2}}$$

where

χ = Concentration of pollutant

t = Time

λ = Decay constant

$T_{1/2}$ = Removal time for one-half of the pollutant

Thus Equation 1 may be modified to read

$$\chi = \frac{Q}{\pi u \sigma_y \sigma_z} \exp\left(-\frac{y^2}{2\sigma_y^2} - \frac{z^2}{2\sigma_z^2}\right) \exp\left(-\frac{0.693t}{T_{1/2}}\right) \quad (2)$$

The half-life or the half residence time of pollutants such as CO, CO_2, and SO_2 are not well known. In urban air pollution models, a value for SO_2 of four to six hours has often been used [2]. Since chemical reaction rates are markedly influenced by temperature, e.g., a doubling for every 10° C rise in temperature, the residence time must also be a function of temperature if chemical reactions are involved.

B. Modification for Elevated Sources and Plume Rise

With the origin of the coordinate system at the ground, but the source at a height, h', Equation 2 becomes

$$\frac{\chi}{Q} = \frac{1}{\pi u \sigma_y \sigma_z} \exp\left(-\frac{y^2}{2\sigma_y^2} - \frac{(z-h')^2}{2\sigma_z^2}\right) \exp\left(-\frac{0.693t}{T_{1/2}}\right) \quad (3)$$

Of course, materials emitted from a stack do not necessarily stay at the same level. The plume may rise because of its buoyancy and

momentum. The height of plume rise, Δh, must be added to the chimney height to result in an effective plume rise, $h = h' + \Delta h$. There are numerous formulas for calculating plume rise [33]. Equation 3 then becomes

$$\frac{\chi}{Q} = \frac{1}{\pi u \sigma_y \sigma_z} \exp\left(-\frac{y^2}{2\sigma_y^2} - \frac{(z-h)^2}{2\sigma_z^2}\right) \exp\left(-\frac{0.693t}{T_{1/2}}\right) \qquad (4)$$

C. Mixing of Pollutant under an Inversion Lid

When the lapse rate in the lowermost layer, i.e., from the ground to about 200 meters, is near adiabatic but a pronounced inversion exists above this layer, the inversion is believed to act as a lid preventing the upward diffusion of pollutants. The pollutants below the lid are assumed to be uniformly mixed. By integrating Equation 4 with respect to z and distributing the pollutants uniformly over a height, H, one obtains

$$\frac{\chi}{Q} = \frac{1}{2\pi u \sigma_y H} \exp\left(-\frac{y^2}{2\sigma_y^2}\right) \exp\left(-\frac{0.693t}{T_{1/2}}\right) \qquad (5)$$

Those few measurements of concentration with height which do exist, do not support the assumption that the concentration is uniform in the lowermost layer. One is tempted to say that the mixing layer thickness, H, may be determined by the height of the inversion; however, during transitional conditions, i.e., at dawn and dusk, the thickness of the layer containing high concentrations of pollutants may differ from that of the layer from the ground to the inversion base.

The thermal structure of the lower layer as well as pollutant concentration as a function of height may be determined by helicopter soundings.

D. The Area Source

When pollution arises from many small point sources such as small dwellings, one may consider the region as an area source. Preliminary work on the Chicago model [16, 17] indicates that contributions to observed SO_2 levels in the lowest tens of feet substantially from dwellings exceeds that emanating from tall stacks such as power generating stacks. For a rigorous treatment, one should consider the emission Q as the emission in units per unit area per second, and then integrate Q along x and along y for the length of the square. Downwind, beyond the area source square, the plume may be treated as originating from a point source. This point source is considered to be at a virtual origin upwind of the area source square. As pointed out by Turner [34], the approximate equation for an area source

$$\frac{\chi}{Q} = \frac{\exp\left(-\frac{y^2}{[2\sigma_y(x_{y_o}+x)]^2} - \frac{(z-h)^2}{2\sigma_z^2}\right)\exp\left(-\frac{0.693t}{T_{1/2}}\right)}{\pi u[\sigma_y(x_{y_o}+x)]\sigma_z}$$

where $\sigma_y(x_{y_o}+x)$ represents the standard deviation of the horizontal crosswind concentration as a function of the distance $x_{y_o}+x$ from the virtual origin. Since the plume is considered to extend to the point where the concentration falls to 0.1 that of the centerline concentration, $\sigma_y(x_{y_o}) = S/4.3$ where $\sigma_y(x_{y_o})$ is the standard deviation of the concentration at the downwind side of the square of side length S. The distance, x_{y_o}, from the virtual origin to the downwind side of the grid square may be determined from Fig. 2, and is that distance for which $\sigma_y(x_{y_o}) = S/4.3$. The distance x is measured from the downwind side of the grid square. Other symbols

have been previously defined.

E. Correction for Variation in Chimney Height

In any given area, chimneys are likely to vary in height above ground, and the plume rises vary as well. The variation of effective stack height may be taken into account in a manner similar to the handling of the area source. To illustrate, visualize the points representing the effective stack height projected onto a plane perpendicular to the ground and parallel both to two opposite sides of the given grid square and to the horizontal component of the wind vector. The distribution of the points on this projection plane would be similar to the distribution of the sources on a horizontal plane.

Based on Turner's discussion [34], the equation for an area source and for a source having a Gaussian distribution of effective chimney heights may be written as

$$\frac{\chi}{Q} = \frac{\exp\left(-\frac{y^2}{2[\sigma_y(x_{y_o}+x)]^2} - \frac{(z-h)^2}{2[\sigma_y(x_{z_o}+x)]^2}\right)\exp\left(-\frac{0.693t}{T_{1/2}}\right)}{\pi u[\sigma_y(x_{y_o}+x)][\sigma_z(x_{z_o}+x)]}$$

where $\sigma_z(x_{z_o}+x)$ represents the standard deviation of the vertical crosswind concentration as a function of the distance $x_{z_o}+x$, from the virtual origin. The value of $\sigma(x_{z_o})$ is arbitrarily chosen after examining the distribution of effective chimney heights and the distance x_{z_o} represents the distance from the virtual origin to the downwind side of the grid square. The value x_{z_o} may be determined from Fig. 3 and represents the distance corresponding to the value for $\sigma_z(x_{z_o})$. The value of x_{y_o} usually differs from that of x_{z_o}. The other symbols retain their previous definition.

In determining the values of $\sigma_y(x_{y_o} + x)$ and $\sigma_z(x_{z_o} + x)$ one must know the distance from the source to the point in question or the receptor. If the wind direction changes within the averaging interval, or if there is a change of wind direction due to local terrain effects, the trajectories are curved. There are several ways of handling curved trajectories. In the Connecticut model, for example, analytic forms for the trajectories were developed. The selection of appropriate trajectory or stream line equations (steady state was assumed) was based on the wind and stability conditions. In the St. Louis model, Turner [35] developed a computer program using the available winds to provide pollutant trajectories. Distances obtained from the trajectories are then used in the Pasquill diagrams such as in Figs. 2 and 3 to determine the values of $\sigma_y(x_{y_o} + x)$ and $\sigma_z(x_{z_o} + x)$.

IX. METEOROLOGICAL MEASUREMENTS

Wind speed and direction data measured by the Weather Bureau were used by most investigators, even though some had a number of stations and towers of their own. New York City had an extensive meteorological wind network consisting of over 100 anemometers as well as pilot balloons to provide information on wind variation with height. Smaller programs made use of one or two anemometers.

Pollutants were measured for periods of one hour, two hours, twelve hours, or twenty-four hours. Twelve and twenty-four hour samples of pollutants such as SO_2 leave much to be desired, since many features of their variations with time are obscured. Further, one often has difficulty in determining a representative wind direction or even a representative wind speed for such a long period.

The total amount of data available varies considerably in the eleven studies. Frenkiel's study was based on data for one month only. A comparatively large amount of data was gathered by Davidson, but even these in truth represent a small sample. The most extensive study is the one carried out by the Argonne National Laboratory and the City of Chicago in which 15-minute readings of SO_2 for eight stations and wind speed and direction for at least thirteen stations are available for a three-year period.

In the application of the mathematical equations, one is required to make numerous arbitrary decisions: for example, one must choose the way to handle the vertical variation of wind with height when a high stack, circa 500 feet, is used as a point source; or how to test changes in wind direction or stability when a change occurs half-way through the one-hour or two-hour measuring period. In the case of an elevated point source, Turner in his St. Louis model, treated the plume as one originating from a point source up to the time of a change in wind direction and as a combination of an instantaneous line puff and a continuous point source thereafter. The occurrence of precipitation presents serious problems since adequate diffusion measurements under these conditions are lacking. Further, the chemical and physical effects of precipitation on pollutants are only poorly understood. In carrying forward a pollutant from a source, one must decide on how long to apply the calculations. For example, if a two-mile per hour wind is present over the measuring grid and a source is ten miles away, must one take account of the transport for a total of five hours.

Determining a representative wind speed and wind direction over

an urban complex with its variety of buildings and other obstructions to the flow is frequently difficult since the horizontal wind field is quite heterogeneous. This is so for light winds, especially during the daytime when convective processes are taking place. With light wind conditions, the wind direction may differ by 180° within a distance of one mile. Numerous wind stations are necessary to depict the true wind field. With high winds, those of the order of 20 mph, the wind direction is quite uniform over a large area so that fewer stations are necessary. It appears that an adequate number of measurements to handle the light wind condition was lacking in all of the studies except the one in New York City.

X. METHODS FOR EVALUATING THE MATHEMATICAL MODEL.

To determine the effectiveness of the mathematical model, validation tests must be applied. These usually include a comparison of observed and calculated values. Validation tests are necessary not only for updating the model because of changes in the source configuration or modifications in terrain characteristics due to new construction, but also for comparing the effectiveness of the model with any other which may be suggested. Of course, the primary objective is to see how good the model really is, both for incident control as well as for long range planning.

A. Scatter Diagrams and Correlation Measures

Of the validation techniques appearing in the literauture, the most common involves the preparation of a scatter diagram relating observed and calculated values (Y_{obs} vs. Y_{calc}). See Fig. 10. The degree of scatter about the 45° line provides a measure of the effectiveness of the model. At times, one finds that a majority of the

points lies either above the line or below the line, indicating systematic errors.

It is useful to determine whether the model is equally effective at all concentration levels. To test this, the calculated scale may be divided into uniform bandwidths and the mean square of the deviations about the 45° line calculated for each bandwidth. Another test for systematic error as a function of bandwidth consists of an examination of the mean of the difference between calculated and observed values for $Y_{calc} > Y_{obs}$ and similarly for $Y_{calc} < Y_{obs}$.

The square of the linear correlation coefficient between calculated and observed values or the square of the correlation ratio for non-linear relationships represent measures of the effectiveness of the mathematical equation. For a linear relationship between the dependent variable, e.g., pollutant concentration, and the independent variables.

$$R^2 = 1 - \frac{S_y^2}{\sigma_y^2} = 1 - \frac{\text{unexplained variance}}{\text{total variance}} = \frac{\sigma_y^2 - S_y^2}{\sigma_y^2} = \frac{\text{explained variance}}{\text{total variance}}$$

where R^2 = the square of the correlation coefficient between observed and calculated values, S_y^2 = the average of the square of the deviations about the regression line, plane, or hyperplane, and σ_y^2 is the variance of the observed values.

B. Contingency Tables

A variation of the scatter diagram is the contingency table shown in Table VIII. To determine whether such a table can be explained by chance, a X-square test may be applied.

Two variations of the contingency table have been found useful [36] as illustrated in Tables IX and X. In the first table,

(Table IX), each entry of Table VIII is divided by the sum of its respective column, and multiplied by 100, e.g., 60 = 9/15 x 100 for the entry in row 2, column 2. The table provides the percentage frequency distribution of the observed values given the forecast concentration value and indicates the fraction of forecasts which were verified.

In Table X, a similar calculation is made, but this time each entry of Table VIII is divided by the sum of its respective row and multiplied by 100. This provides information on the relative effectiveness of the model as a function of the observed value. It is especially important to see how well the model works for each portion of the observed range of concentration values. A useful model should be particularly effective for high concentration values.

One must consider the magnitude of the range of variables. If the range of observed pollution values is small or the distribution about the mean is small because only a small sample was used, misleading results may be obtained. If the range is small because the pollution values are always small and vary but little, then there is no need for sophisticated calculations. Forecasting presents no problem, and the citizens are fortunate.

C. Skill Scores

Another model validation measure is the Heidtke skill score [36] which may be expressed as

$$\frac{\text{No. of Correctly Calculated Values Minus No. of Expected Hits}}{\text{Total No. of Calculated Values Minus No. of Expected Hits}}$$

or

$$\text{Skill Score} = \frac{V - E}{T - E}$$

V = Number of calculations which are verified

E = Expected hits according to some criterion

T = Total number of calculations

The expected value E may be calculated in a number of different ways depending on whether the forecast equation is compared to pure chance, persistence, climatology, or some other forecast scheme.

The skill score is subject to manipulation since there is leeway in deciding what constitutes a correct calculated value. In practice, one indicates that concentrations will fall within a given bandwidth rather than that a specified value will occur. The width of the band selected subjectively, therefore, determines the magnitude of the skill score.

A cruder way of presenting the effectiveness of a model is to indicate the ratio of hits within a given band to the total number of calculations, e.g., 8/10 of the calculations fell within 0.03 ppm of the observed value.

D. Effectiveness of Model as a Function of a Particular Variable

Let us assume that the calculation based on the model was verified if the calculated value and the observed value differ by 5 pphm or less. We may then determine the per cent of calculated values which exceeded, were verified or were less than the values in the observed band. Also, we may stratify the data in accordance with a particular variable, e.g., wind speed. Then for each wind speed group interval, we may compute the per cent of calculated values which were greater than, were verified, or were less than the observed band

values. When a plot is made of these percentages as a function of wind speed intervals as seen in Fig. 11, we have an indication of the relation between the effectiveness of the model and a particular variable. Further, the data may be stratified according to two or more variables such as would be the case if the computation of Fig. 11 were carried out for data with the wind direction in the 270-315° sector, i.e., stratification by wind direction as well as speed. Stratification may be extended to include stability and temperature. Multiple stratification is limited by the amount of data available since too small a number of cases in each cell of the multidimensional space may result.

If the observed concentration is a function of several variables, viz, wind speed, wind direction, temperature, and stability, then by stratifying the data, the effect of each variable may be studied. For example, consider only data where the wind direction ranges from 270° to 315° and the atmosphere is very stable, then we may plot observed concentration versus temperature for a wind speed band of 1-4 mph. On the same graph, a similar plot can be made for calculated concentrations so that the observed and calculated values may be compared. Graphs can be made for other combinations of variables.

A comparison of observed and calculated values of the oxides of nitrogen for each hour of the day is shown in Fig. 12. No other data stratification is involved in this figure.

E. Spatial and Temporal Variation of Pollutants - Isopleth Charts

The pollutant concentrations as well as the meteorological variables are functions of the three space coordinates, x, y, and z,

and time, t. Thus we have a five-dimensional system

$$F(x,y,z,t,\emptyset) = 0$$

where $\emptyset$ is a meteorological or pollutant variable. By holding two dimensions fixed, let us say t and z, we may draw isopleths of $\emptyset$ as a function of x and y in a horizontal plane. A vertical cross-section may be obtained by holding y and t constant.

Davidson [11] has made detailed soundings of SO_2 and temperature using a helicopter to obtain vertical cross sections. Although time, t, was not constant, the variables were assumed to vary slowly with time. A case study as shown in Fig. 13 provides an enlightening picture of the layering of warm air.

Isopleths on a horizontal plane may be drawn for observed values with calculated values plotted at the stations or drawn for calculated values with the observed values plotted. Another possibility is to draw isopleths of ratios of observed to calculated values. See Fig. 14. Such charts are valuable since they call attention to areas of high concentrations as well as to the shape of these areas, e.g., elongated, diffuse, or circular. The location and magnitude of the maximum is clearly indicated. When one plots a number of such isopleth charts, each for a different wind direction, the effect of large sources on the pollution pattern becomes evident.

Thus there are a number of ways of presenting the results of a comparison between observed and calculated values and of calculating measures of merit. In the last analysis the effectiveness of the model must be judged by how well it works to provide the needed information whether it be for day-to-day control, for incident alerts,

or for long range planning.

XI. CONCLUDING REMARKS

An examination of the work covered in this report forces one to the conclusion that there is ample room for development.

Inadequacies and shortcomings exist in our assessment of each of the components of the mathematical urban air pollution model.

A. The Source Inventory

For large metropolitan areas, one finds that the inventory obtained by the usual methods such as questionnaires is often out of date upon its completion. A continual updating is necessary. However, in a receptor-oriented model, the requirement for a detailed source inventory is relaxed. Further, by developing a receptor-oriented "anomaly" model, one may further reduce the error resulting from inadequate source information. In the "anomaly" type model, changes in the dependent variable over a given period are calculated. This interval may be one, two, four, or six hours.

B. Pollutant Measurements

An examination of Table II, shows that pollutant measurements were sparse. It is necessary to remember that the distribution of any contaminants is a function of space and time. With a heterogeneous distribution of sources in space and the pronounced variation in source strength with time, one can hardly expect a few stations to describe adequately the distribution of the contaminant sources. Further, in the models to date, no group has measured the variation of the pollutant in the vertical continuously. In the New York study, a helicopter provided this kind of information, but at best, it was fragmentary. Also, the averaging time is important. A one-

hour sample or even a two-hour sample will bring out the diurnal effects quite well; however, twenty-four hour samples do not.

C. Meteorological Measurements

The amount of weather data is inadequate. Since the concentrations at a given receptor are markedly affected by the wind direction, the wind field must be known. One must consider not only the horizontal variation of wind speed and direction near the surface, but also the variation with height, the shear. The orientation of the mean air flow over a city has an additional effect. When the winds are perpendicular to the long axis of a rectangular-shaped city then the residence time of materials over the city is relatively short. If the winds are along the long axis, there will be greater accumulations on the downwind side.

In most of the studies, information on the stability was obtained only indirectly. Measurements of the vertical variation of temperature with height was only rarely obtained. In the New York study, the helicopter did obtain such information.

Measurements of the mixing layer depth was for the most part absent. This information can be obtained by remote probing techniques such as lidar or radar, by balloons, or by aircraft or helicopters. However, the mixing layer depth is an essential parameter in determining the volume over which the material will be mixed, and is of importance in forecasting levels of atmospheric concentrations.

D. The Mathematical Algorithm

Most of the studies have been based on the simple Gaussian model with suitable corrections such as those for the variation of stack

heights, plume rise, or removal rates of the contaminant. Changes in the wind direction or stability during the measuring interval were either ignored or treated crudely. The selection of adequate values for the adjustable parameters was well nigh impossible because of the lack of good measurements.

E. Validation Techniques

The literature shows that efforts to validate the effectiveness of a model are fraught with difficulties. The calculated values of skill scores may be of questionable significance since they involve considerable subjectivity in the selection of the bandwidth representing a forecast hit or in the technique for calculating the expected values. Further, skill scores based on the entire range of pollutant values are not completely useful since it may be trivial to forecast low values of pollutant concentration, but may be extremely important to know when high values will occur to prevent damage to property or the onset of respiratory difficulties. The model should therefore be geared for maximum effectiveness at the high end of the scale, e.g., levels of SO_2 exceeding 0.5 ppm. Similar problems are encountered in forecasting low ceilings or frost since only one end of the scale of variables is of interest.

Acceptable statistical procedures were at times violated. Where concentration data from several stations were available, these were lumped together to provide a large sample. This is in general unacceptable especially where pronounced heterogeneity in the areal distribution of concentration existed. Further, in time series of pollutant concentrations, autocorrelation effects must be considered in assessing the number of independent measurements for use

in significance determinations.

XII. FUTURE CONSIDERATIONS

If mathematical modeling is to be effective, it is essential that information be available on the space-time distribution of both the pollutant and the necessary meteorological variables. By considering concentration changes with time and using the receptor-oriented approach, one may minimize the influence of the source inventory, but in the last analysis, source inventory information is necessary for any model. In the validation procedure, one must consider the occurrence of systematic errors, i.e., readings consistently too high or too low compared to the calculated values. Similarly, large deviations between calculated and observed values should be carefully investigated. The selection of an appropriate sampling time is most important.

In conclusion, although the efforts made to date on the problem are commendable, the results are still not as good as is desired. The continued effort in the development of an urban air pollution model is necessary, and hopefully will provide the needed tools for handling urban air pollution problems.

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TABLE CAPTIONS

Table I Investigators, locations and pollutants of urban air pollution models.

Table II Investigators, amounts of data, period of study and publication dates of urban air pollution models.

Table III Investigators, monitoring stations and monitoring grids of urban air pollution models.

Table IV Investigators, time per sample, grid size and effective plume rise of urban air pollution models.

Table V Basic Equations.

Table VI Key to stability categories. (After Pasquill as given by Turner [34].)

Table VII Tabulation prediction scheme.

Table VIII Contingency table for SO_2 concentration forecasts.

Table IX Per cent of time each forecast concentration of SO_2 occurred as indicated.

Table X Per cent of time each observed category of SO_2 concentration was forecast as indicated.

TABLE I INVESTIGATORS, LOCATIONS AND POLLUTANTS OF URBAN AIR POLLUTION MODELS

INVESTIGATORS	LOCATION	POLLUTANT
Frenkiel	Los Angeles, Calif.	Number of contaminants including ozone. (All not specified)
Turner	Nashville, Tennessee	SO_2
Clarke	Cincinnati, Ohio	SO_2, NO_x
Fortak	Bremen, Germany	SO_2
Hilst & Bowne	Ft. Wayne, Indiana	Fluorescent Particles
Pooler	St. Louis, Missouri	Fluorescent Particles
Miller & Holzworth	Washington, D. C. Los Angeles, Calif. Nashville, Tennessee	NO NO^x SO_2^x
Davidson	New York, New York	SO_2
Koogler Sholtes Danis & Harding	Jacksonville, Fla.	SO_2
Panofsky & Prasad	Johnstown, Pa.	Particulates
Hilst Badgley Yocum & Bowne	Connecticut	Hydrocarbons, CO, NO_x, SO_2, & particulates

TABLE II

INVESTIGATORS, AMOUNTS OF DATA, PERIOD OF STUDY AND PUBLICATION DATES OF URBAN AIR POLLUTION MODELS

INVESTIGATOR	DATE OF PUBLICATION	PERIOD OF STUDY	NO. OF OBSERVATIONS OF POLLUTANTS
Frenkiel	April 1956	Sept. 1956	
Turner	February 1964	Oct. 1958 - Mar. 1959	1036 24-hr readings 2710 2-hr readings
Clarke	September 1964	Jan. - May 1962	33 days
Fortak	February 1966	Jan. - Dec. 1962	
Hilst & Bowne	July 1966	Mar. 1964 - Feb. 1966	21 experiment periods (days) 70 releases
Pooler	December 1966	May 1963 - Mar. 1965	43 experiments
Miller & Holzworth	January 1967	a. Los Angeles, May 1963 b. Nashville, Oct. 1958 - Mar. 1959 c. Washington, D. C., 1962 - 1964	36 test days 31 test days 41 test days
Davidson	March 1967	1963 - 1967	9 experiment periods 5 days per period
Koogler Sholtes Danis & Harding	April 1967	Dec. 1965 - Jan. 1966	12 days, 111 observations
Panofsky & Prasad	June 1967	Oct. 1964 - Nov. 1964 July 1965 - Aug. 1965 Oct. 1965 - Nov. 1965 Jan. 1966 - Feb. 1966	

INVESTIGATOR	DATE OF PUBLICATION	PERIOD OF STUDY	NO. OF OBSERVATIONS OF POLLUTANTS
Hilst Badgley Yocum & Bowne	Cctober 1967	(Source inventory - 1967.)	none

TABLE III INVESTIGATORS, MONITORING STATIONS AND MONITORING GRIDS OF URBAN AIR POLLUTION MODELS

INVESTIGATOR	NUMBER OF MONITORING STATIONS	MICROMETEOROLOGICAL MEASUREMENTS
Frenkiel	1	Used available published data, no special measurements.
Turner	32 stations making 24-hour measurements 7 stations making 2-hour measurements	Wind speed and direction at 10 meters - four stations
Clarke	1	
Fortak	none	Weather Service - Bremen Airport, no special instrumentation
Hilst & Bowne	25 sequential samplers 250 rotorod samplers 10 Gelman tape samplers 13 rotorods on 244-meter tower 23 rotorods on tethered barrage balloon 4 rotorods on 61-meter tower	Wind and temperature measurements at ten stations: six in the city and four in the rural surroundings. One 244-meter tower with temperature and wind measurements at 12.2, 30.5, 61, 91 and 213 meters; one 61-meter tower with wind and temperature measurements at 15.2, 22.9, 30.5, 47.2 and 53 meters; two wiresondes and one modified radiosonde; one aircraft to measure turbulence and also temperature by conventional and infrared means.
Pooler	60 rotorod samplers 30 membrane filter samplers 10 drum-pulsed samplers	Three stations at periphery of city with aerovanes and hygrothermographs on KMOX-TV tower; Three levels for measurements of wind, temperature, and vertical temperature gradient. Wind measurements with pilot balloons and also at tracer release site. Free and tethered radiosonde soundings, tetroon soundings

INVESTIGATOR	NUMBER OF MONITORING STATIONS	MICROMETEOROLOGICAL MEASUREMENTS
Miller & Holzworth	Los Angeles, 9 NO_x stations Nashville, 7 SO_2 stations Washington, 1 CAMP station	Weather Bureau - surface and upper air sounding of temperature and wind for each city.
Koogler Sholtes Danis & Harding	11	Five wind stations, 1 TV tower for temperature at 100, 200, 300, 450, and 750 ft.
Davidson	32 fixed ground stations 3 mobile ground stations 1 helicopter	Over 100 anemometers, pibals and helicopter
Panofsky & Prasad	10	Two 150-ft. TV towers for wind and temperature. One 75-ft. tower for wind. Two additional anemometers - airway station data.
Hilst Badgley Yocum & Bowne	none	Weather Bureau stations and Department of Defense stations in Connecticut and adjoining states.

TABLE IV TIME PER SAMPLE, GRID SIZE, AND EFFECTIVE PLUME RISE

INVESTIGATOR	TIME PER SAMPLE (HRS.)	GRID (MILES)	EFFECTIVE PLUME HEIGHT
Frenkiel	---	---	---
Turner	24 2	9 x 11 mile monitoring grid 17 x 16 inventory grid	20 meters
Clarke	2-hr values used to obtain 24-hr averages	Irregular source grid Single monitoring station Computing grid: 1. 22.5 sectors of a circle with monitoring station at center and radius 1 km. 2. 22.5 annular sectors bounded by arcs of concentric circles with 1 km and 4 km radii; also for 4 and 10 km radii.	30 meters - SO_2 20 meters - NO_x
Fortak	---	Source grid: 1 km square subdivided into 100 sub-squares. Computing grid: 480 x 800 meters rectangularly arranged in a 50 grid x 50 grid network.	Domestic - 15 m Small emitters - 25 m (less than 1 kgm/hr)
Hilst & Bowne	10 Gelman tape samplers - 5 min 25 sequential samplers - 30 min Rotorod samplers - variable (depends on wind speed)	5 parallel lines, 1/2 mile between sampling, 50 samples per line.	---
Pooler	1	Group I arcs: 0.5, 2, and 4.5 mi with 6° spacing Group II arcs: 1.25, 2.5, and 5 mi with 6° spacing Group III arcs: 10 mi with 3° spacing In later experiments, the 4.5 and 5 mi had 3° spacing.	---

INVESTIGATOR	TIME PER SAMPLE (HRS.)	GRID (MILES)	EFFECTIVE PLUME HEIGHT
Miller & Holzworth	Los Angeles: 2-hr. Nashville: 2-hr. Washington, D. C.: 4-hr.	Los Angeles: Details of Monitoring Grid not given. Same as Turner's for 2-hr. samples. Single CAMP station	---
Davidson	1	1-mi. square, 50 x 50 sq. mi.	Space heating/hot water 30.5 m.
Koogler Sholtes Danis & Harding	24	1-mi. square, 15 x 15 sq. mi.	$\Delta h = \frac{1.5V_s d+aQ_H}{u}$ at 2000 m For distance from source > 2000 m $\Delta h = \frac{1.5V_s d+aQ_H}{u} \frac{x^{2/3}}{2000}$
Panofsky & Prasad	12 24	---	---
Hilst Badgley Yocum & Bowne	---	5000-ft. squares over area of State of Connecticut	

TABLE V BASIC EQUATIONS

1. Frenkiel

Equation not given

2. Turner

$$\frac{\chi}{Q} = \frac{1}{u\pi(\sigma_y+402)\sigma_z} \exp\left(-\frac{1}{2}\frac{y^2}{(\sigma_y+402)^2} - \frac{1}{2}\frac{(z-h)^2}{\sigma_z^2}\right)\exp\left(-\frac{0.693}{T_{1/2}}t\right)$$

3. Clarke

$$\frac{\chi}{Q} = \frac{2}{u\sqrt{2\pi}\sigma_z((\pi/8)x)} \exp\left(-\frac{1}{2}\frac{z^2}{\sigma_z^2}\right)\exp\left(-\frac{0.693}{T_{1/2}}t\right)$$

where x = distance from source

4. Fortak

Gaussian

5. Hilst & Bowne

$$D(x-x_o,\ 0) = \frac{Q}{\sqrt{2\pi}u(\sigma_{z_o}+a(x-x_o))} \exp\left(-\frac{1}{2}\frac{z_o^2 e^{-2\lambda(x-x_o)}}{(\sigma_{z_o}+a(x-x_o))^2}\right)$$

$D(x-x_o,\ 0)$ = dosage at a distance from line source of $x-x_o$

σ_{z_o} = standard deviation of concentration at release level

a and λ = constants

6. Pooler

$$\frac{\chi}{Q} = \frac{1}{\pi u(\sigma_y+80)(\sigma_z+30)} \exp\left(-\frac{1}{2}\frac{y^2}{(\sigma_y+80)^2} - \frac{h^2}{2(\sigma_z+30)^2}\right)$$

7. Miller & Holzworth

$$\frac{\chi}{Q_A} = \frac{u}{s}\int_{50}^{t_L}\int_{50}^{t_L}\frac{2dtdt}{\sqrt{2\pi}\sigma_z} + \int_{t_L}^{t_s}\int_{t_L}^{t_s} 1/L\ dt\ dt$$

$(\chi/Q_A) = \frac{\chi \text{ observed}}{Q_A \text{ apparent}}$ and $Q_A = (a-bT).10^{-6}$

χ = average concentration

Q_A = area source strength

t_L = time for plume to reach mixing layer height (L)

t_s = time of travel from most distant source

s = distance from edge of city

T = temperature, °F

a and b = constants

8. Davidson

   Gaussian

9. Koogler, Sholtes, Danis & Harding

$$\frac{\chi}{Q} = \frac{1}{u\pi(\sigma_y+402)\sigma_z} \exp\left(-\frac{1}{2}\frac{y^2}{(\sigma_y+402)^2} - \frac{1}{2}\frac{(z-h)^2}{\sigma_z^2}\right)\exp\left(\frac{0.693}{T_{1/2}}t\right)$$

10. Panofsky & Prasad

   1. $\chi = \frac{2Q}{\sqrt{2\pi}uw\sigma_z}$

   2. $\chi = \frac{a}{uR_v} \Sigma \frac{Q}{wy^p}$

   3. $\sigma_z = b\sigma_\theta x^p$

      w = width of valley floor

      R_v = range of vertical angle of bivane

      p $\sim$ 1 in neutral cases

      p > 1 in unstable cases

      a and b = constants

      σ_θ = standard deviation of azimuth angle fluctuations

11. Hilst, Badgley, Yocum & Bowne

$$\frac{\chi}{Q} = \frac{1}{\pi\sigma_y\sigma_z u} \exp\left(-\frac{1}{2}\frac{y^2}{\sigma_y^2} - \frac{h^2}{2\sigma_z^2}\right)$$

TABLE VI

KEY TO STABILITY CATEGORIES

Surface Wind Speed (at 10 m), m sec^{-1}	Day			Night	
	Incoming Solar Radiation			Thinly Overcast or $\geq$ 4/8 Low Cloud	$\leq$3/8 Cloud
	Slight	Moderate	Slight		
< 2	A	A-B	B		
2-3	A-B	B	C	E	F
3-5	B	B-C	C	D	E
5-6	C	C-D	D	D	D
> 6	C	D	D	D	D

The neutral class, D, should be assumed for overcast conditions during day or night.

TABLE VIII

CONTINGENCY TABLE FOR SO_2 CONCENTRATION FORECASTS

Observed SO_2 Conc. (ppm)	Forecast SO_2 Concentrations (ppm)			Total
	<0.3	0.3-0.5	>0.5	
< 0.3	6	2	2	10
0.3-0.5	3	9	4	16
> 0.5	7	4	5	16
Total	16	15	11	42

TABLE VII

TABULATION PREDICTION SCHEME

Season: Dec., Jan., Feb. Precipitation: No. TAM Station # Period of Data: Jan. 1, 1966 - Dec. 31, 1967

Wind Direction Degrees	Hour of Day (CST)	Wind Speed mph	Temperature °F	Stability °C/100m	Percentile Values of SO_2 Concentrations (ppm) Min.	10	25	50	75	90	95	98	99	Max.	No. of Cases
300-350	08-11	4-7	10-19	> 2	0.10	.12	.15	.20	.35	.50	.85	1.00	1.20	1.50	85
300-350	08-11	4-7	10-19	1.9-0.0	0.08	.10	.13	.15	.30	.40	.70	.90	1.10	1.20	90
300-350	08-11	4-7	20-29	> 2	0.05	.10	.12	.15	.20	.30	.35	.40	.50	.70	92
300-350	08-11	4-7	20-29	1.9-0.0	0.05	.08	.10	.11	.12	.15	.15	.20	.25	.35	81

TABLE IX

PER CENT OF TIME EACH FORECAST CONCENTRATION OF SO_2 OCCURRED AS INDICATED

Observed SO_2 Conc. (ppm)	Forecast SO_2 Concentrations (ppm)		
	<0.3	0.3-0.5	>0.5
< 0.3	37	13	18
0.3-0.5	19	60	37
> 0.5	44	27	45
Total	100	100	100

TABLE X

PER CENT OF TIME EACH OBSERVED CATEGORY OF SO_2 CONCENTRATION WAS FORECAST AS INDICATED

Observed SO_2 Conc. (ppm)	Forecast SO_2 Concentrations (ppm)			Total
	<0.3	0.3-0.5	>0.5	
< 0.3	60	20	20	100
0.3-0.5	19	56	25	100
> 0.5	44	25	31	100

FIGURE CAPTIONS

Figure 1 Schematic diagram of an urban air pollution model.

Figure 2 Variation of σ_y as a function of downwind distance from a source. Stability classes A-F are explained in Table VI. (After Turner [34]).

Figure 3 Variation of σ_z with downwind distance from the source. Stability classes A-F are explained in Table VI. (After Turner [34]).

Figure 4 Example of a source inventory map.

Figure 5 Schematic diagram of calculation techniques for source-oriented model. Sources are located at A, B, C, and D of source inventory grid. A section of the monitoring grid is given by squares 15, 16 and 17. The concentration enclosed by the 0.6 ppm isopleth of source B and the 0.3 ppm isopleth of source D contribute a concentration exceeding 0.9 ppm for square 15. See hatched area.

Figure 6 Greater Cincinnati area showing standard emission areas in the form of sectors of the innermost circle or annular sectors of the other circles. (After Clarke [4]).

Figure 7 Relative concentrations $(\frac{\chi}{Q})$ as a function of wind speed (u), mixing depth (H), and stability classes for ground level sources. The stability classes 1-7 are analogous to the classes A-F discussed previously. (After Clarke [32]).

Figure 8 SO_2 concentration (ppm) vs. time of day for the spring season, March, April, May of 1966 and 1967. Chicago Air Pollution Control Telemetered Automatic Monitoring Station No. 6. No precipitation was occurring. The 50th, 90th, 95th, and 100th percentile curves are shown.

Figure 9 SO_2 concentration (ppm) vs. wind direction for the spring season, March, April, May of 1966 and 1967. Chicago Air Pollution Control Telemetered Automatic Monitoring Station No. 6. No precipitation was occurring. The 50th, 90th, 95th, and 100th percentile curves are shown.

Figure 10 Scatter diagram showing calculated 24-hour SO_2 concentrations vs. observed 24-hour SO_2 concentrations in pphm. Numbers refer to number of observations or number of points at the indicated position of the chart. (After Turner [2]).

Figure 11 Accuracies of calculations within ± 1 pphm vs. time of day. (After Turner [2]). No. of cases shown near top of chart.

Figure 12 Average diurnal calculated and observed values of oxides of nitrogen. (After Clarke [14]).

Figure 13 Vertical and horizontal temperature distribution over rural/urban areas on July 14, 1964. Winds are mostly from the west at about 5 mph. From Westchester to Heliport the section is approximately NNW to SSE and from Heliport to Brooklyn College section is NNW to SSW. Shaded area indicates isothermal inversion layers. (After Davidson [11]).

Figure 14 Observed and computed SO_2 concentrations for January 20, 1966. (After Koogler [9]).

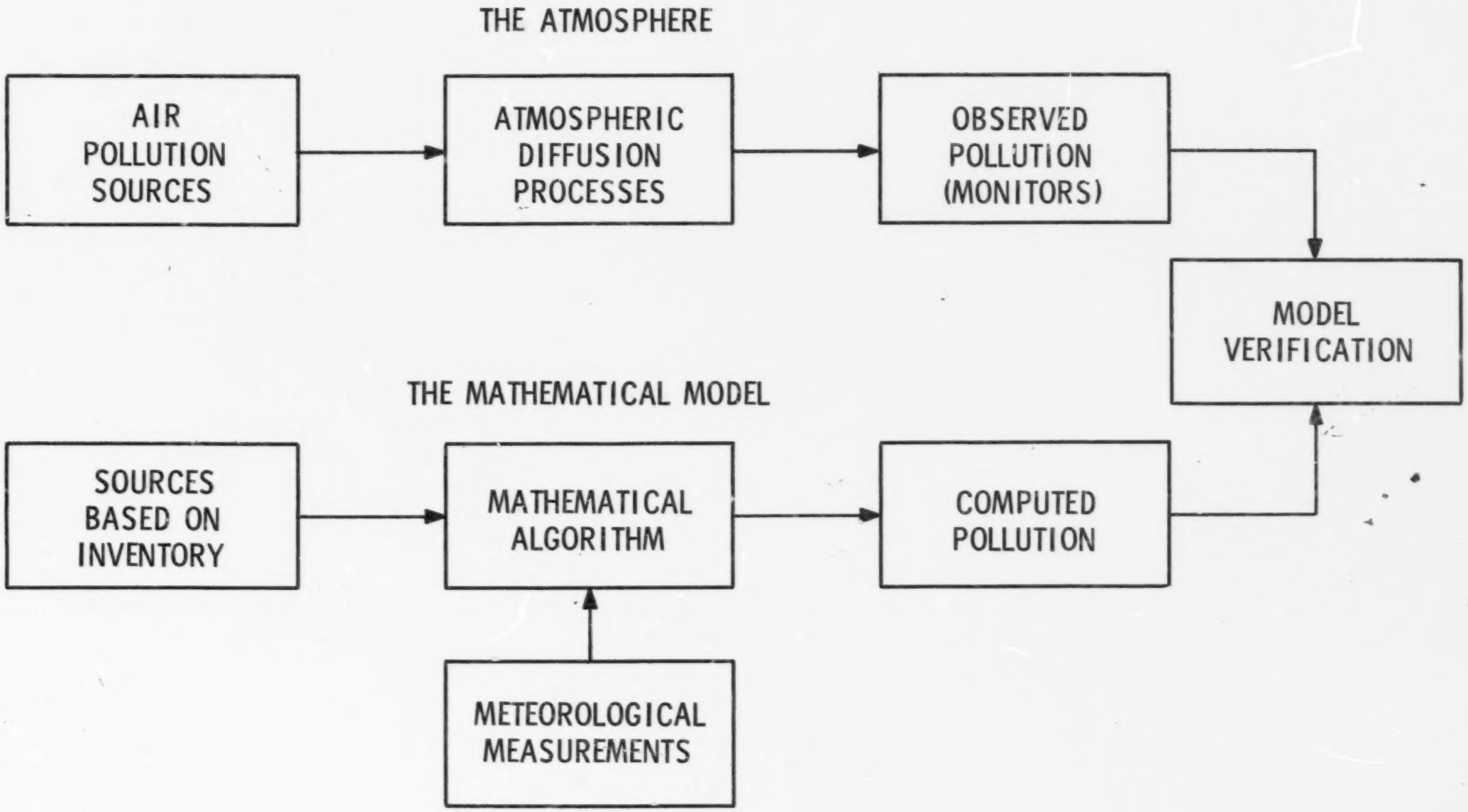

Fig. 1. Schematic Diagram of an Urban Air Pollution Model

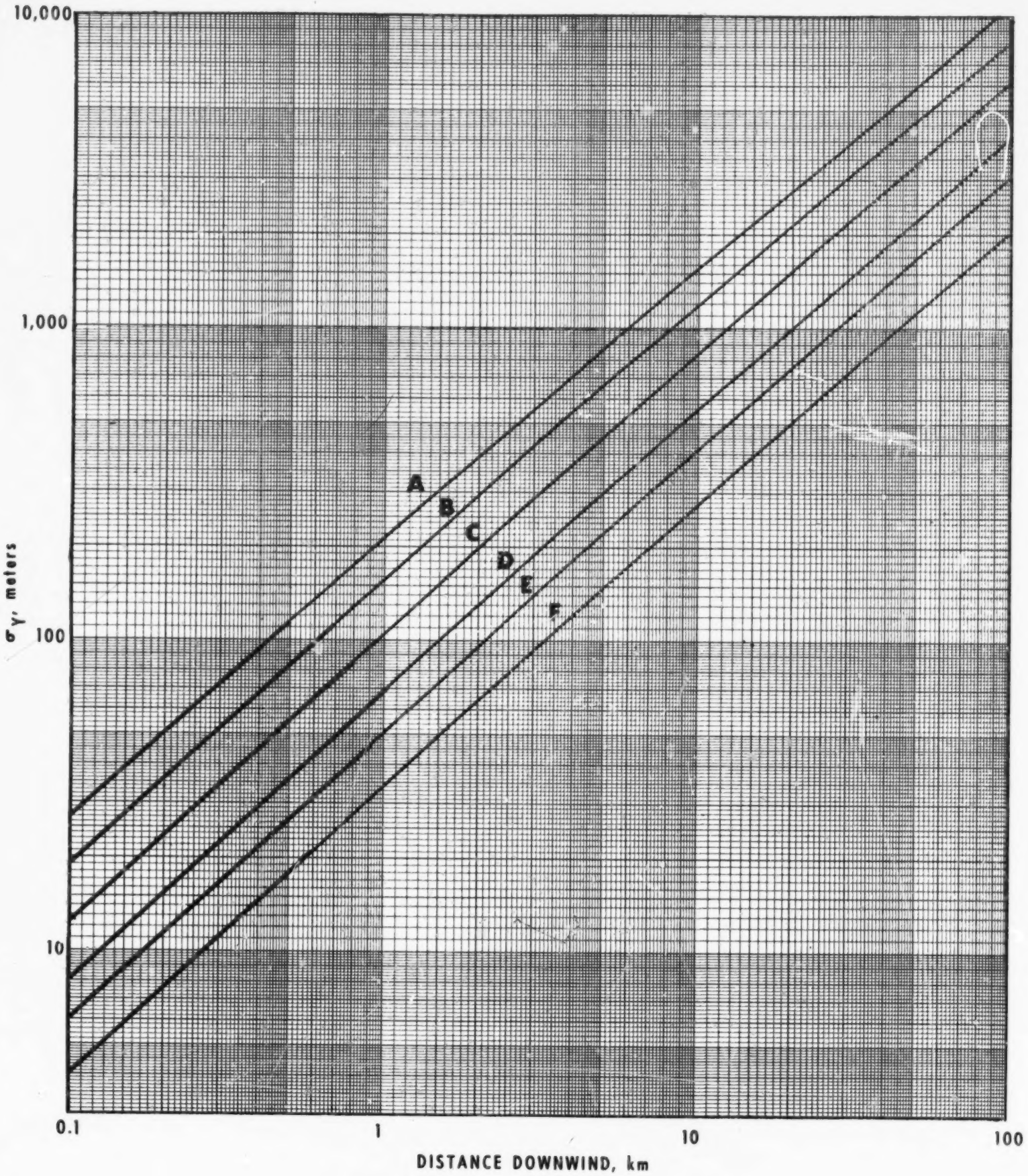

Fig. 2. Variation of σ_y as a Function of Downwind Existance from a Source. Stability Classes A-F are Explained in Table VI.

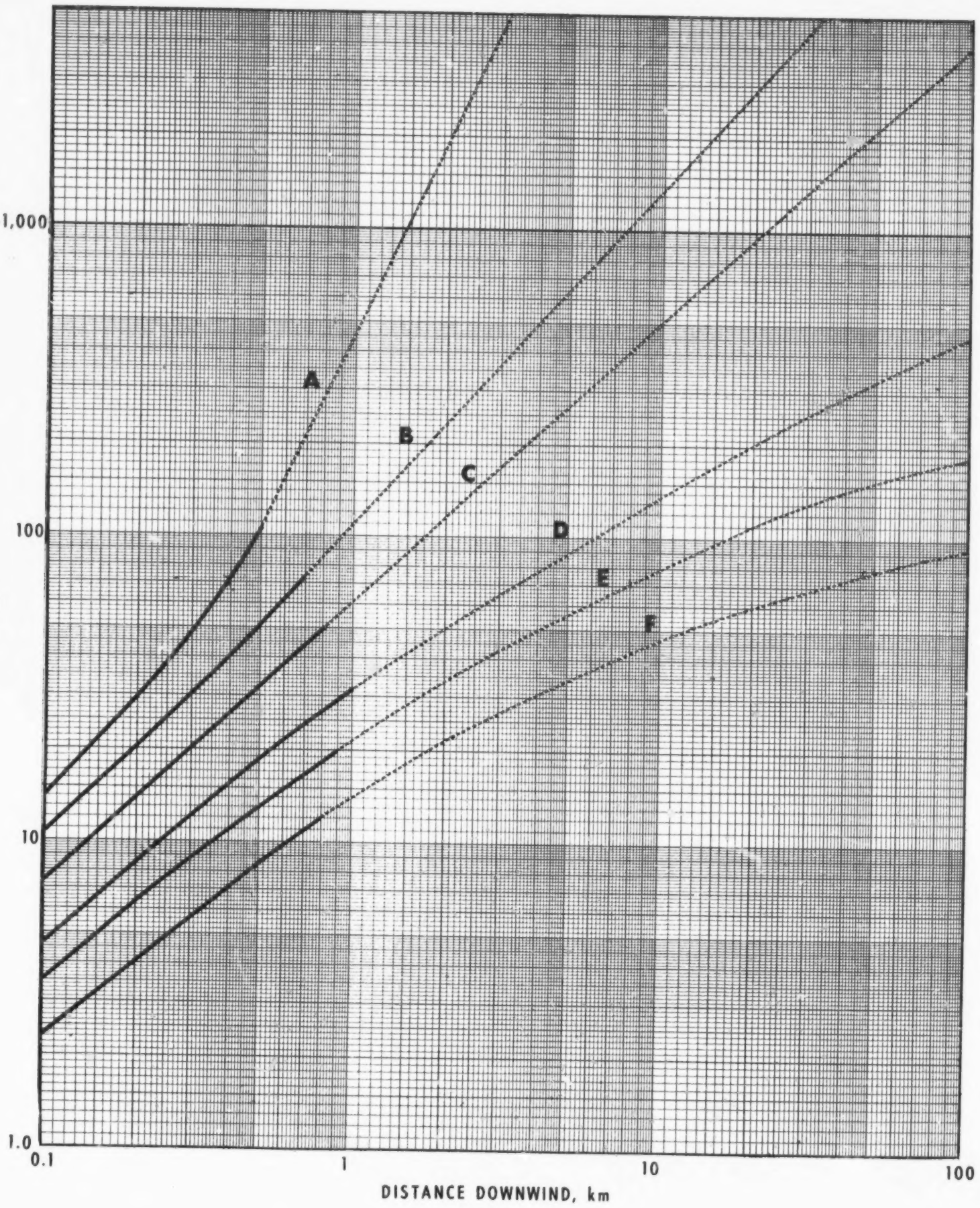

Fig. 3. Variation of σ_z with Downwind Distance from the Source. Stability Classes A-F are Explained in Table VI.

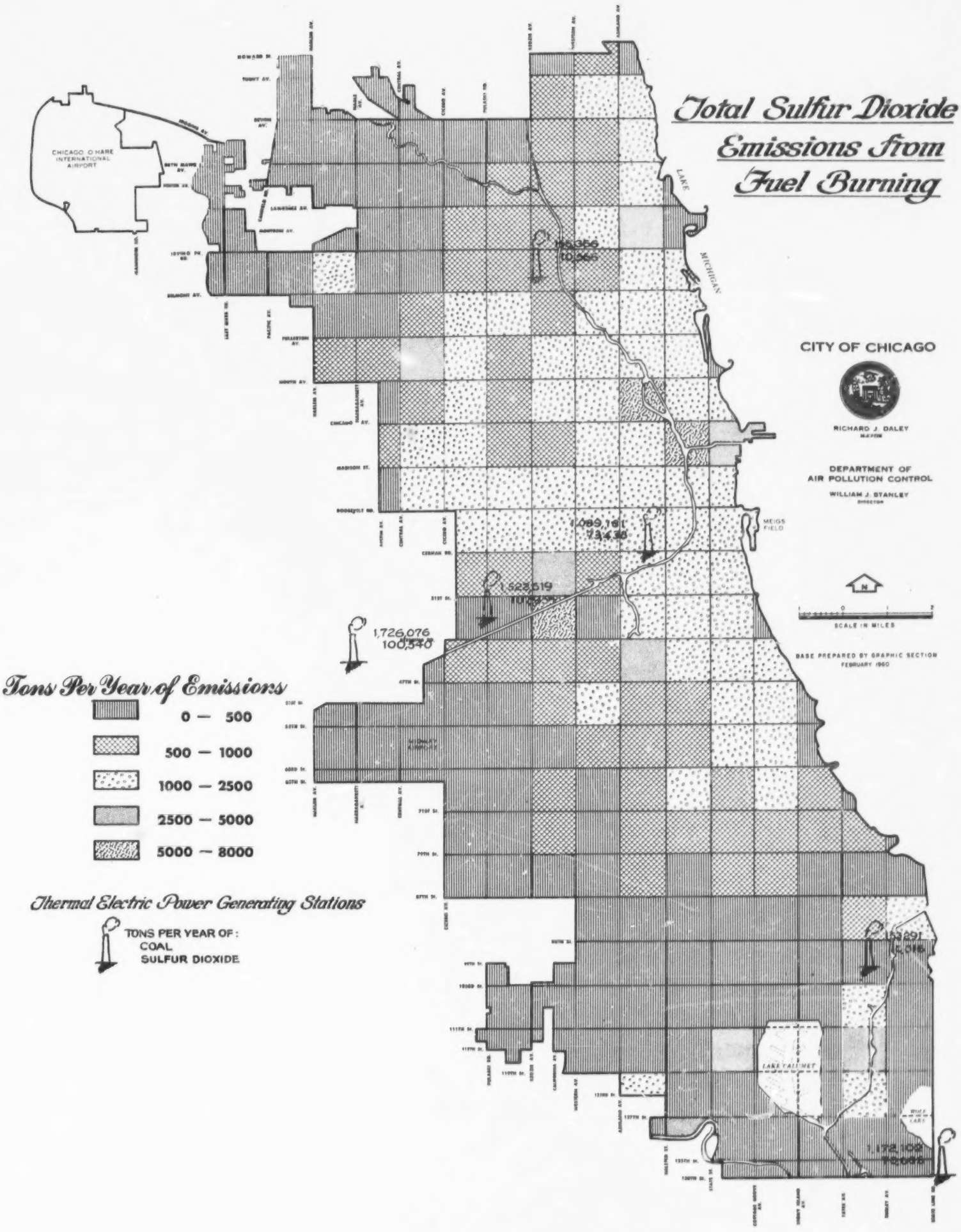

Fig. 4. Example of a Source Inventory Map.

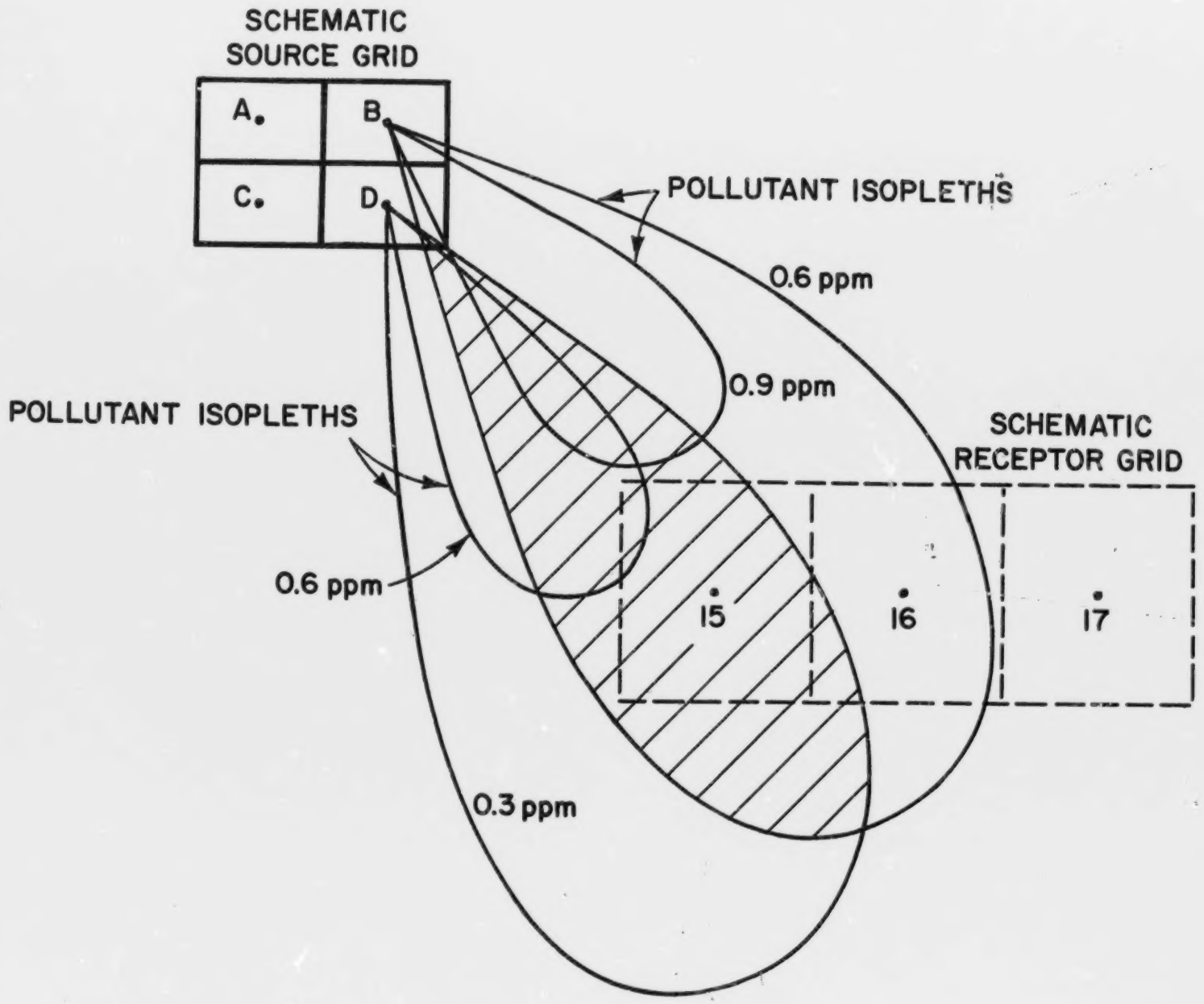

Fig. 5. Schematic Diagram of Calculation Techniques for Source-oriented Model. Sources are Located at A, B, C and D of Source Inventory Grid. A Section of the Monitoring Grid is Given by Squares 15, 16 and 17. The Concentration Enclosed by the 0.6 ppm Isopleth of Source B and 0.3 ppm Isopleth of Source D Contribute a Concentration Exceeding 0.9 ppm for Square 15. See Hatched Area.

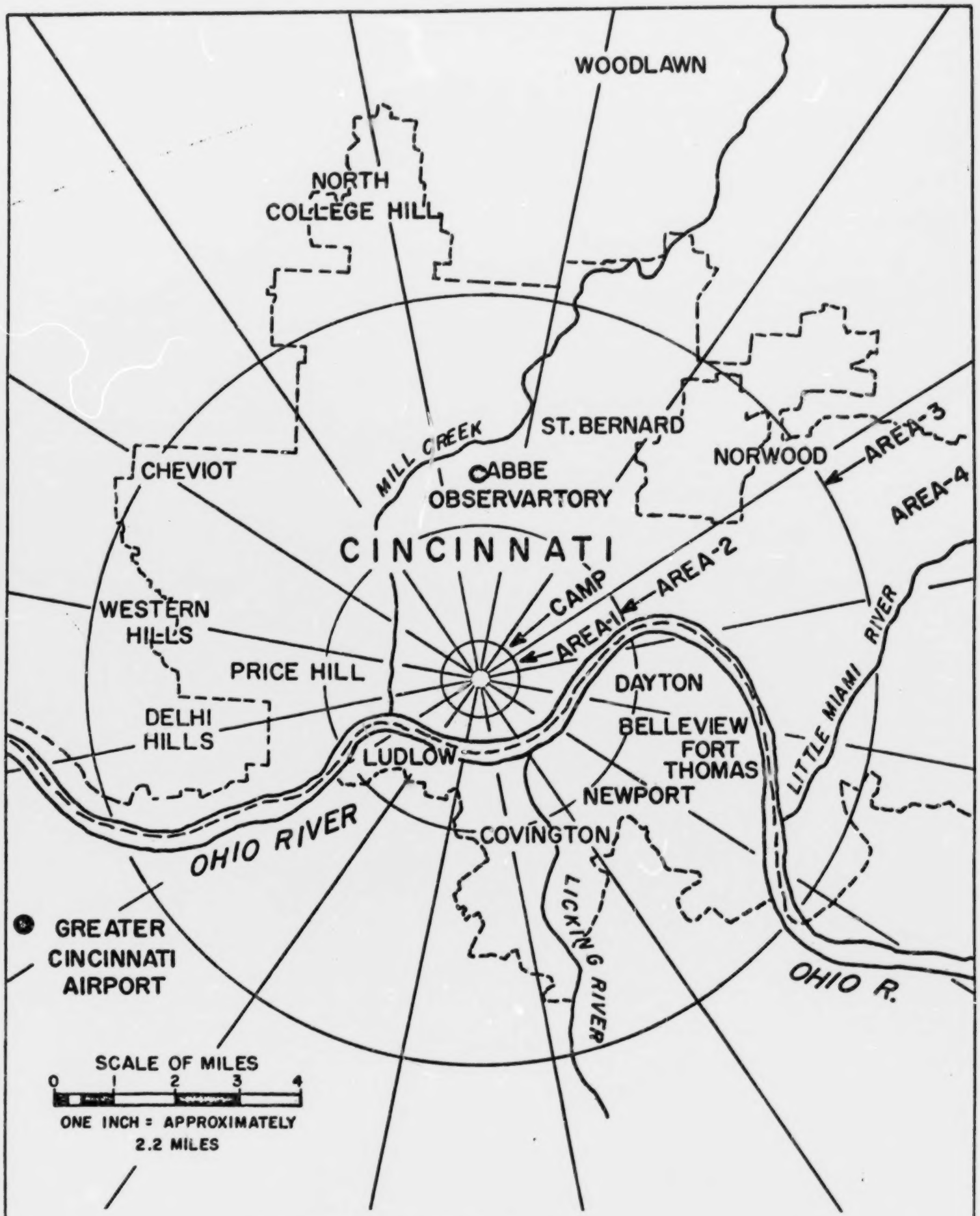

Fig. 6. Greater Cincinnati Area Showing Standard Emission Areas in the Form of Sectors of the Innermost Circle or Annular Sectors of the other Circles.

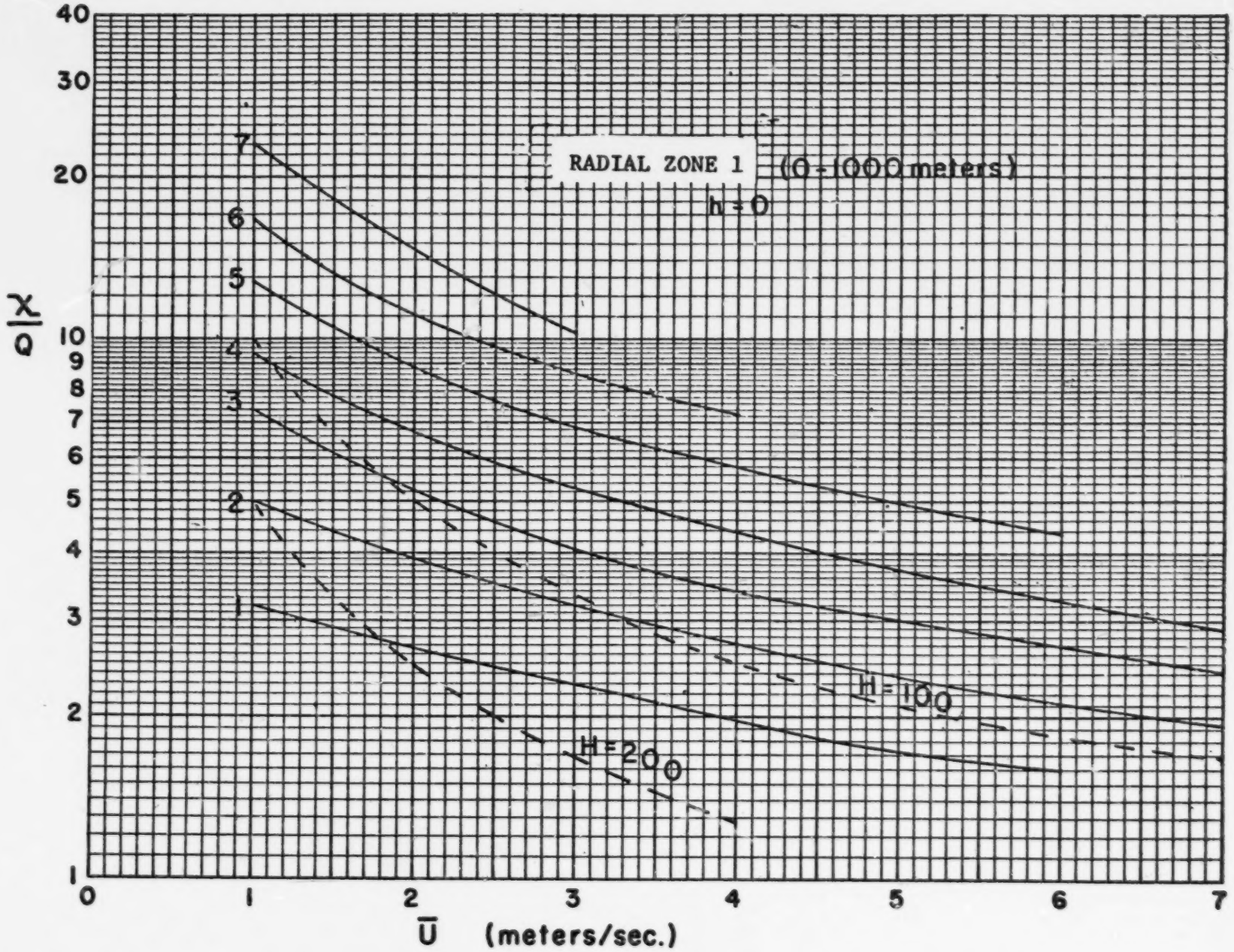

Fig. 7. Relative Concentrations (χ/Q) as a Function of Wind Speed (u), Mixing Depth (H), and Stability Classes for Ground Level Sources. The Stability Classes 1-7 are Analogous to the Classes A-F Discussed Previously.

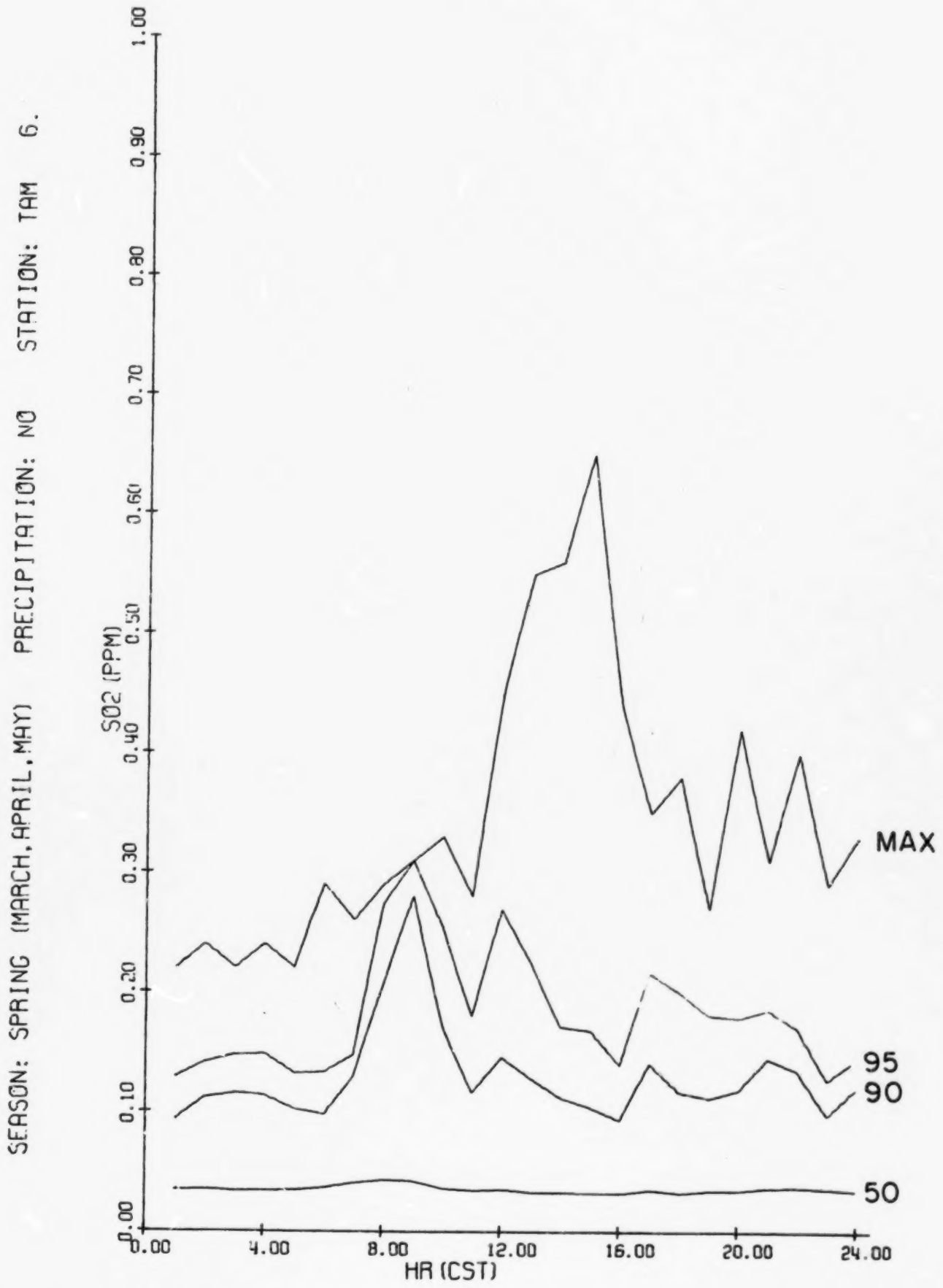

Fig. 8. SO_2 Concentration (ppm) vs. Time of Day for the Spring Season, March, April, May of 1966 and 1967. Chicago Air Pollution Control Telemetered Automatic Monitoring Station No. 6. No Precipitation was Occurring. The 50th, 90th, 95th and 100th Percentile Curves are shown.

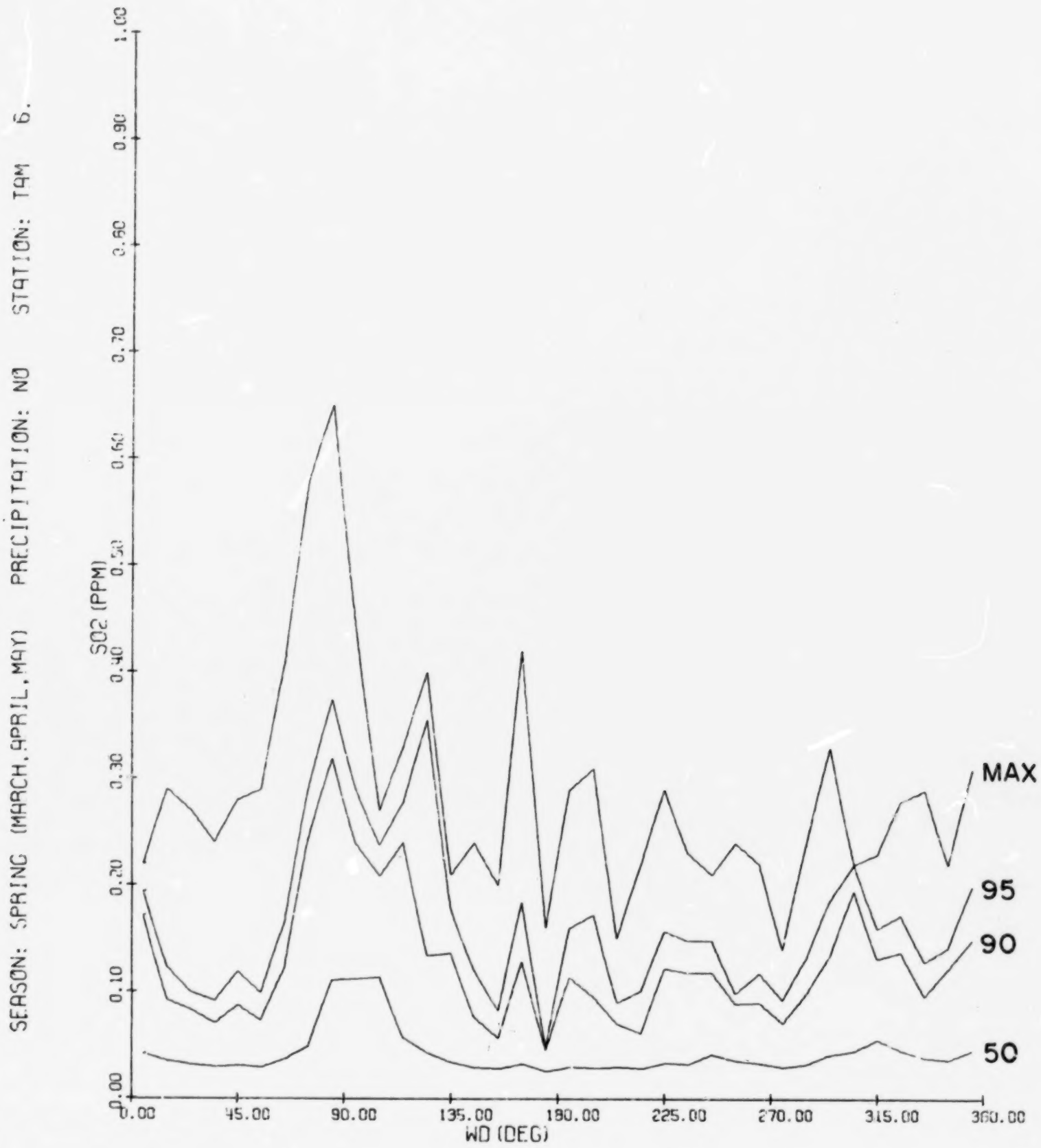

Fig. 9. SO_2 Concentration (ppm) vs. Wind Direction for the Spring Season, March, April, May of 1966 and 1967. Chicago Air Pollution Control Telemetered Automatic Monitoring Station No. 6. No Precipitation was Occurring. The 50th, 90th, 95th and 100th Percentile Curves are shown.

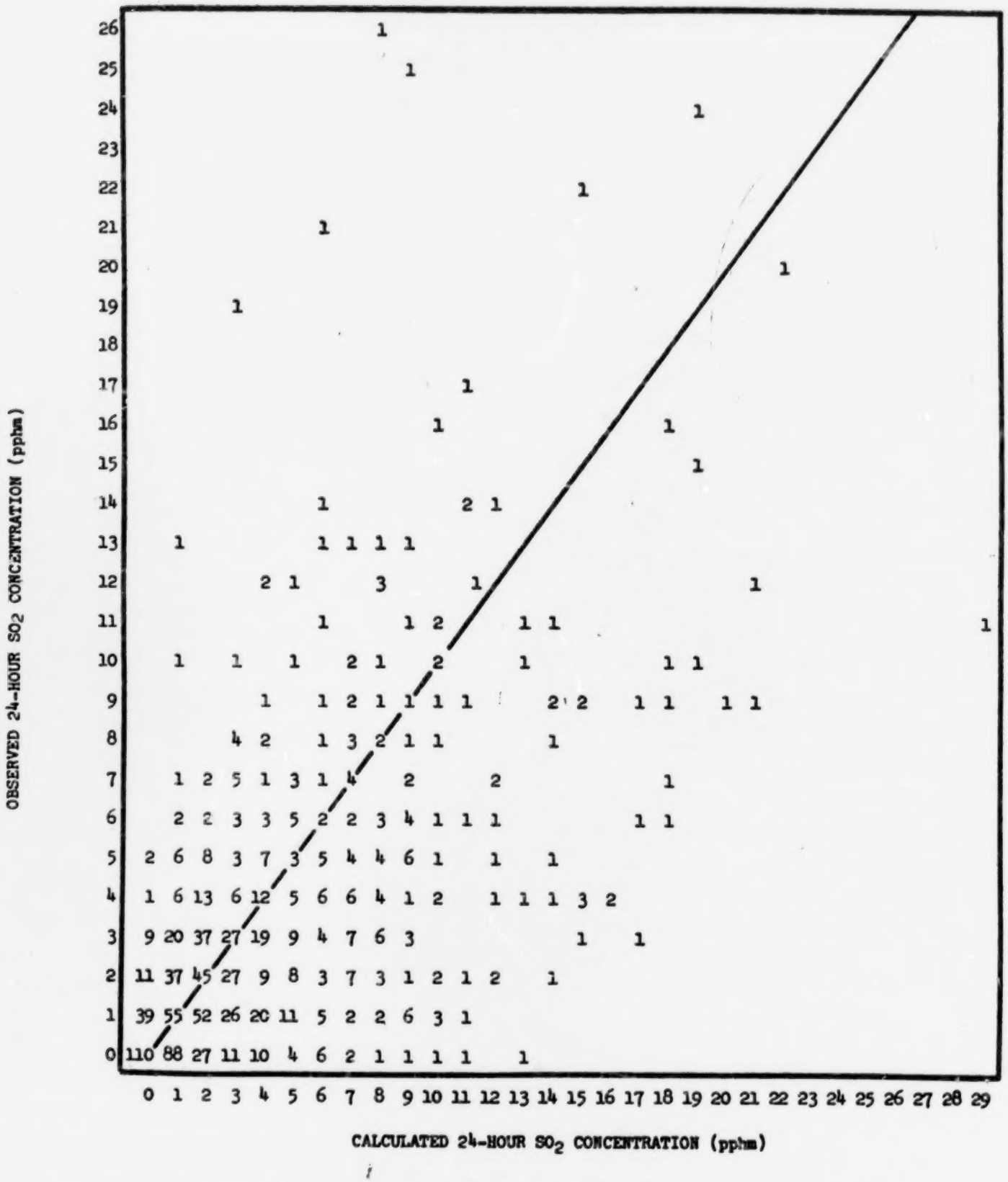

Fig. 10. Scatter Diagram showing Calculated 24-Hour SO_2 Concentrations vs. Observed 24-Hour SO_2 Concentrations in pphm. Numbers refer to Numbers of Observations or Number of Points at the Indicated Position of the Chart.

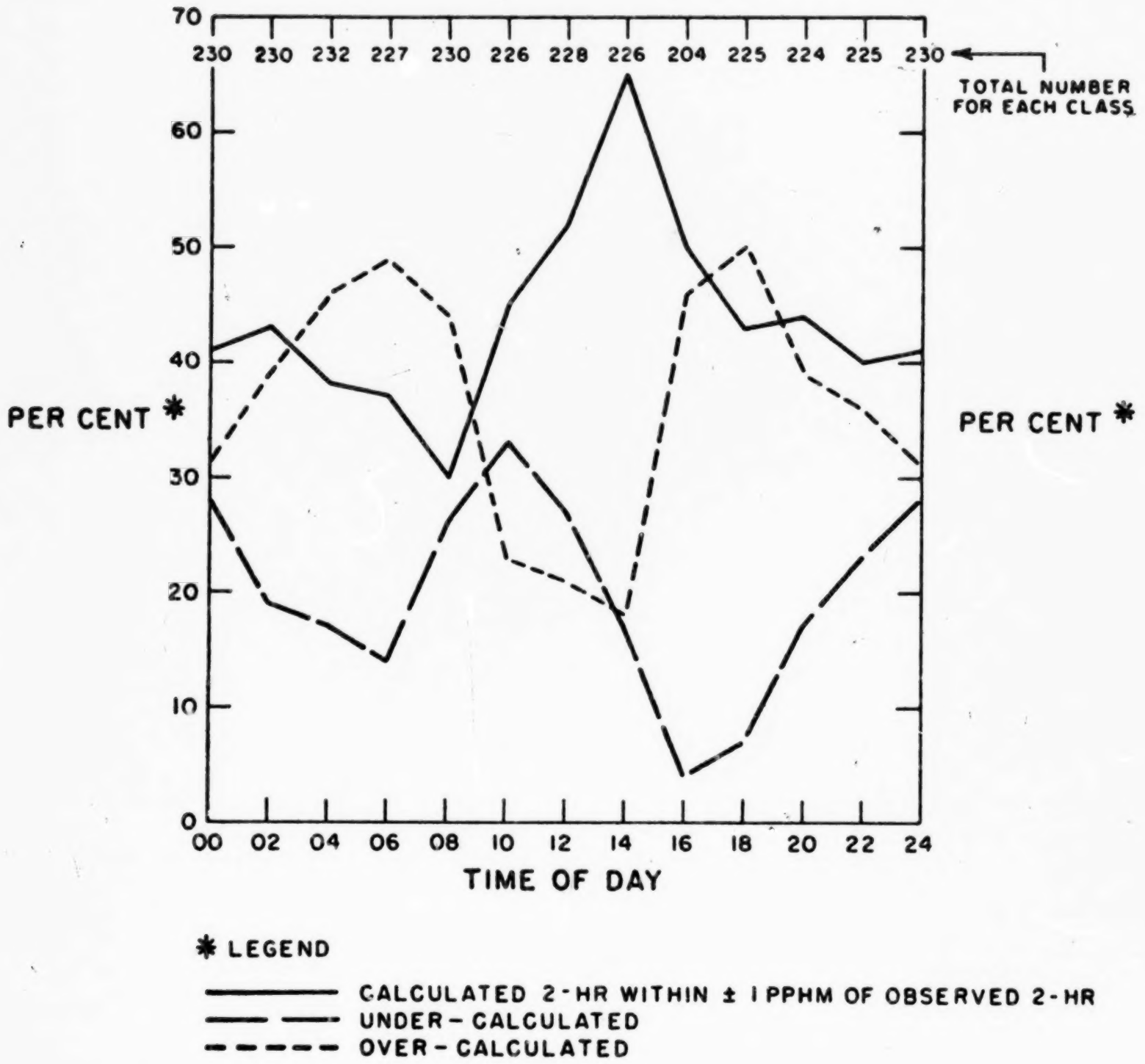

Fig. 11. Accuracies of Calculations within ±1 pphm vs. Time of Day. Number of Cases shown near Top of Chart.

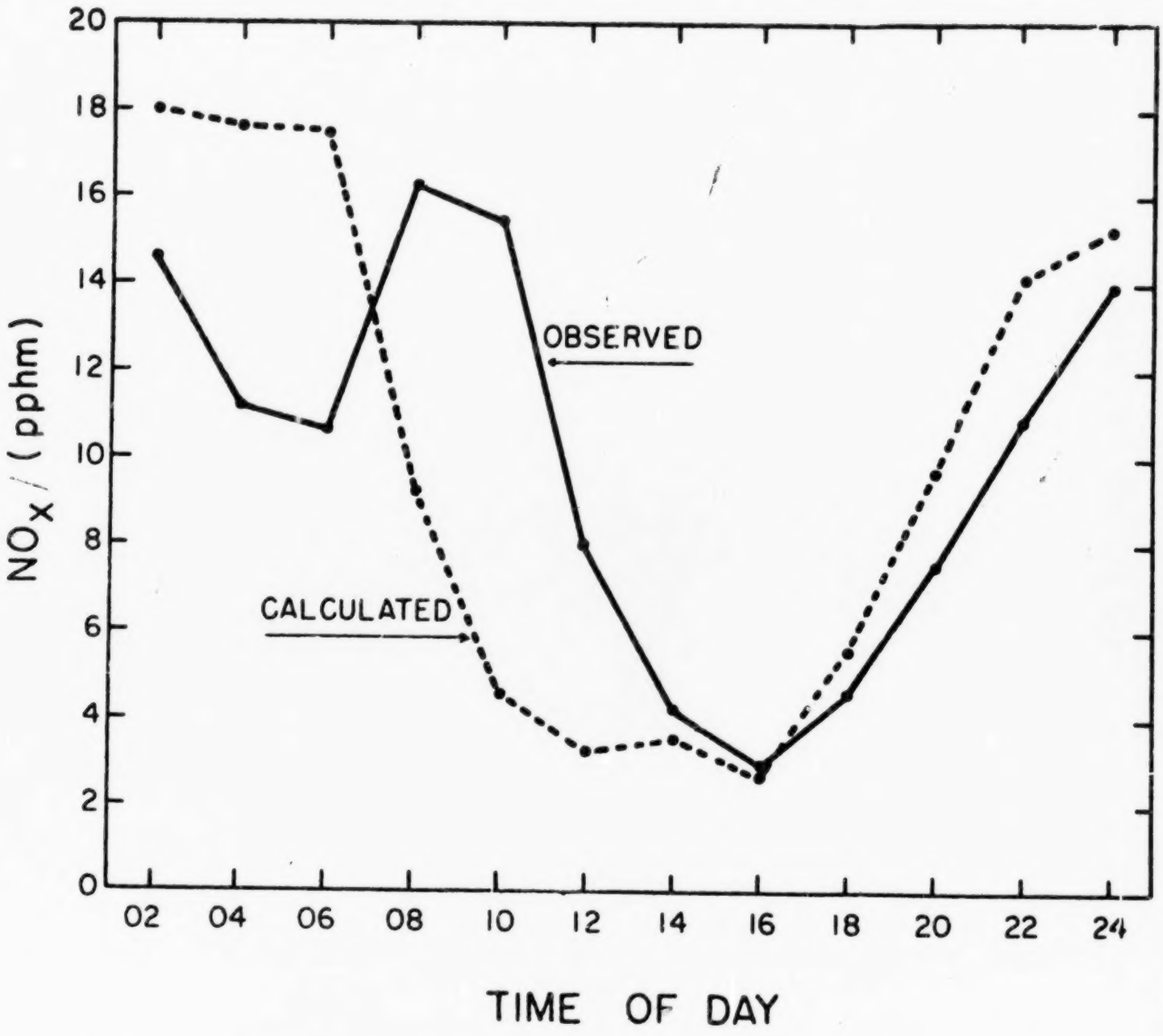

Fig. 12. Average Diurnal Calculated and Observed Values of Oxides of Nitrogen.

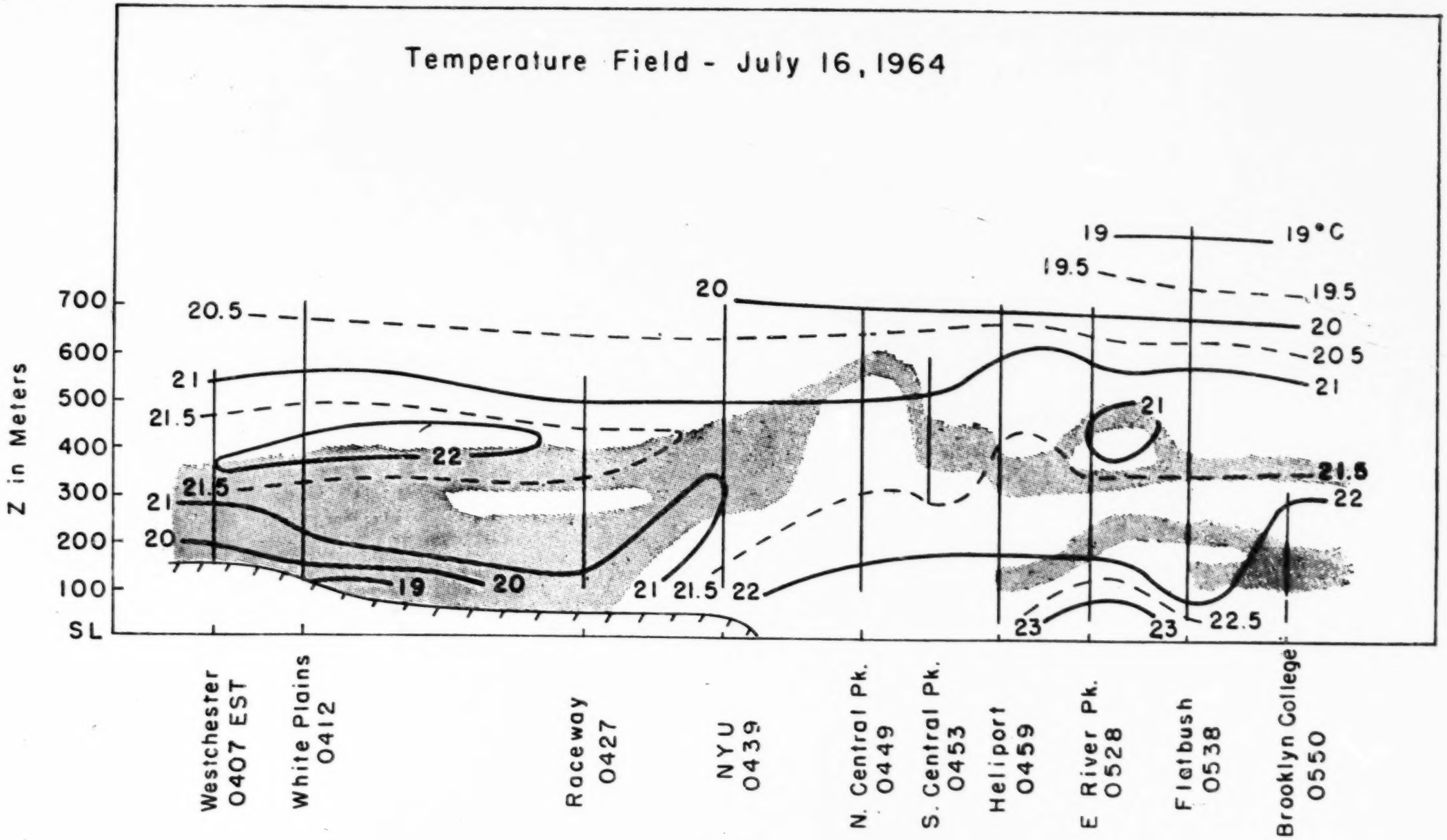

Fig. 13. Vertical and Horizontal Temperature Distribution over Rural/Urban Areas of New York on July 14, 1964. Winds are mostly from the West at about 5 mph. From Westchester to Heliport the Section is Approximately NNW to SSE and from Heliport to Brooklyn College Section is NNW to SSE. Shaded Area Indicates Isothermal Inversion Layers.

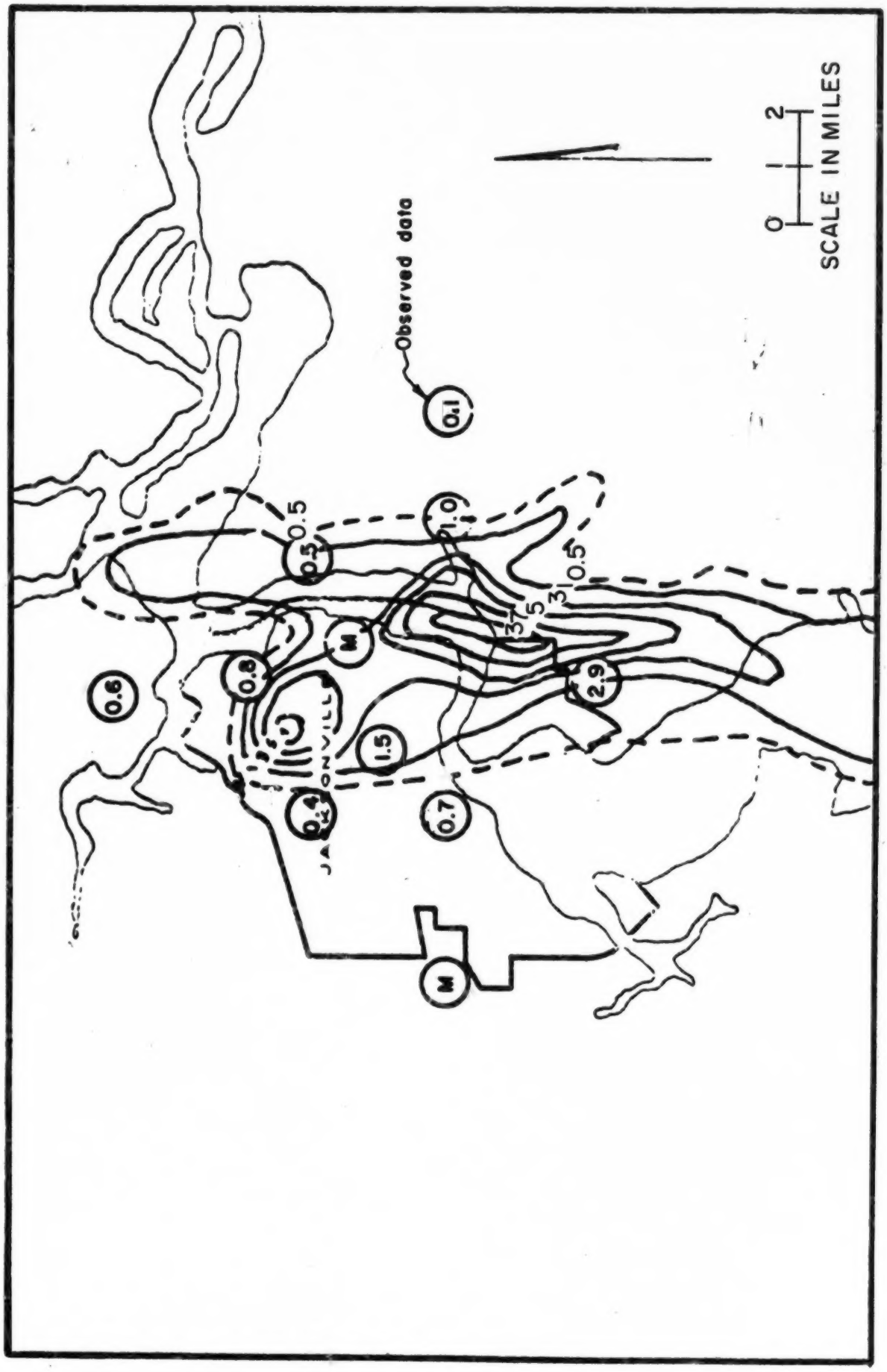

Fig. 14. Observed and Computed SO_2 Concentration for January 20, 1966, Jacksonville, Fla.